

Fig. 2

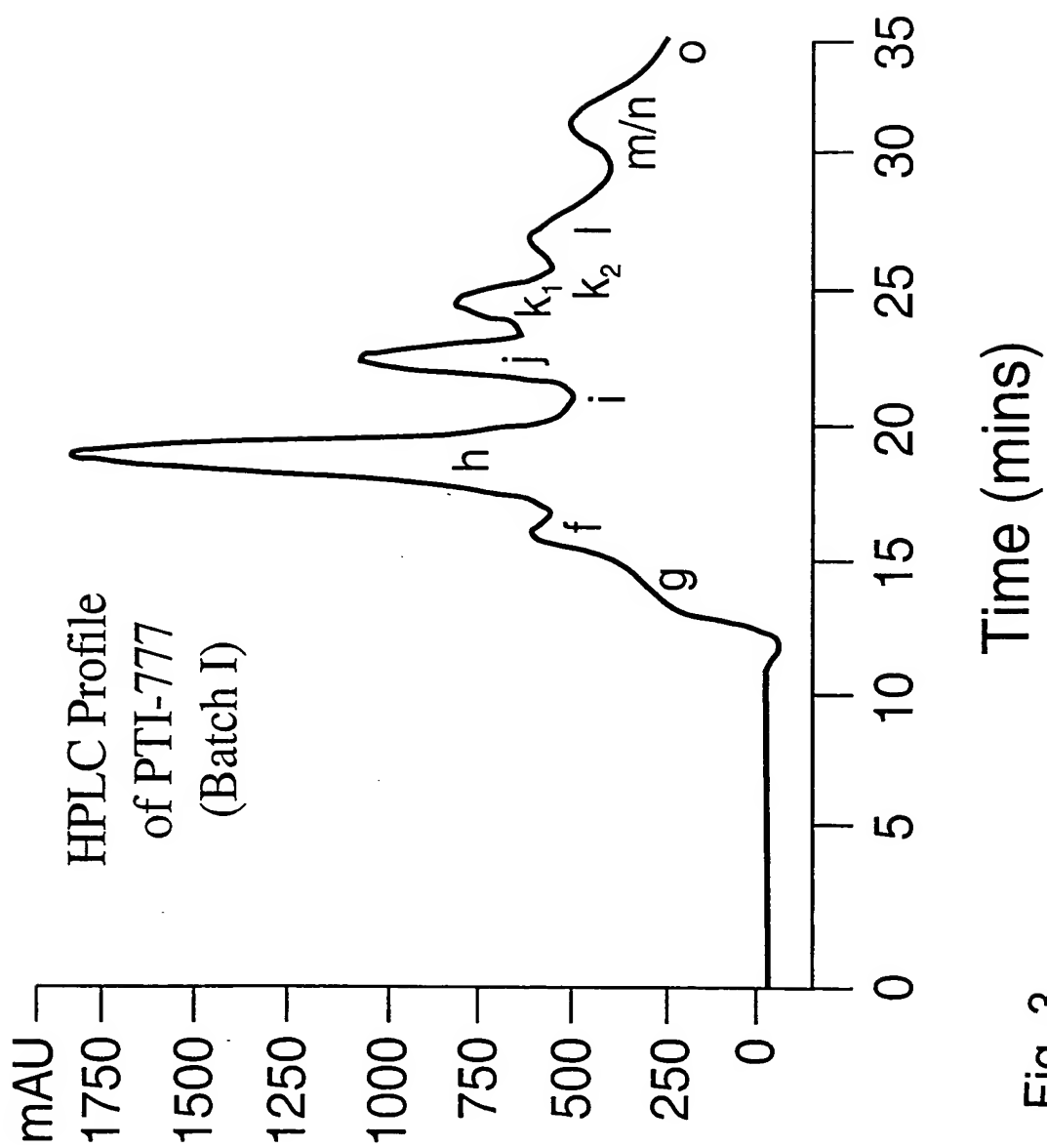
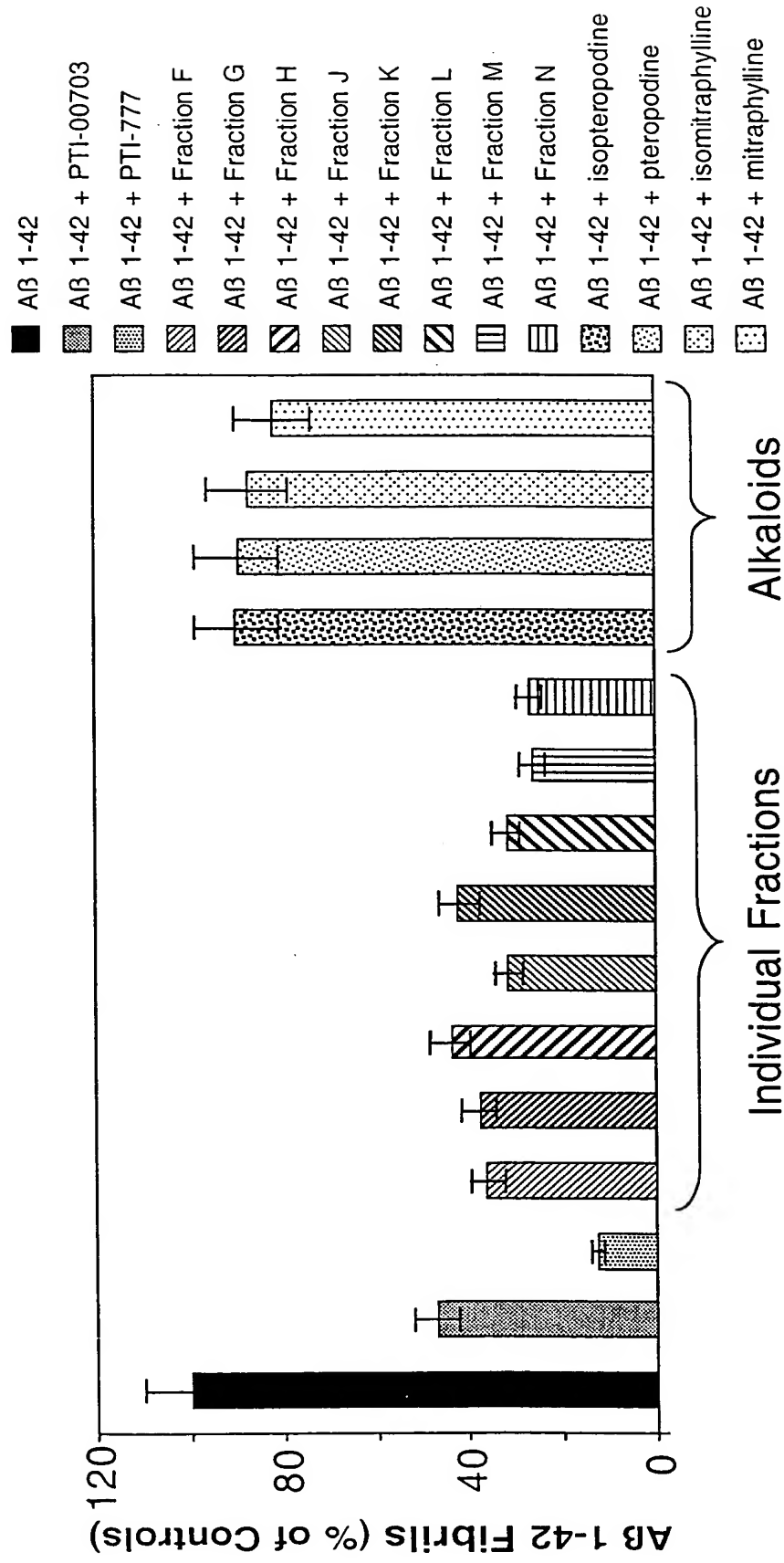


Fig. 3



**Treatment Groups**

Fig. 4



Fig. 5A

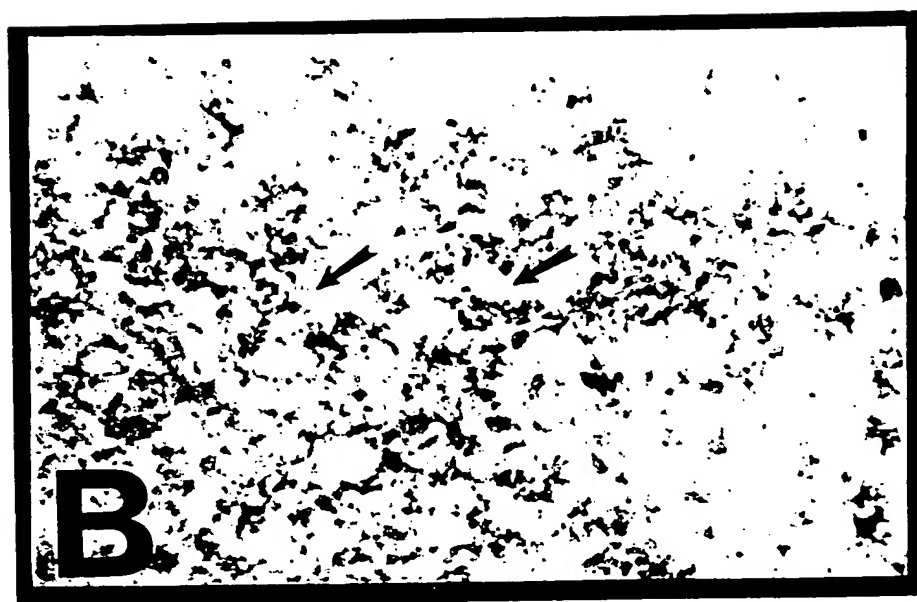


Fig. 5B



Fig. 5C



Fig. 5D

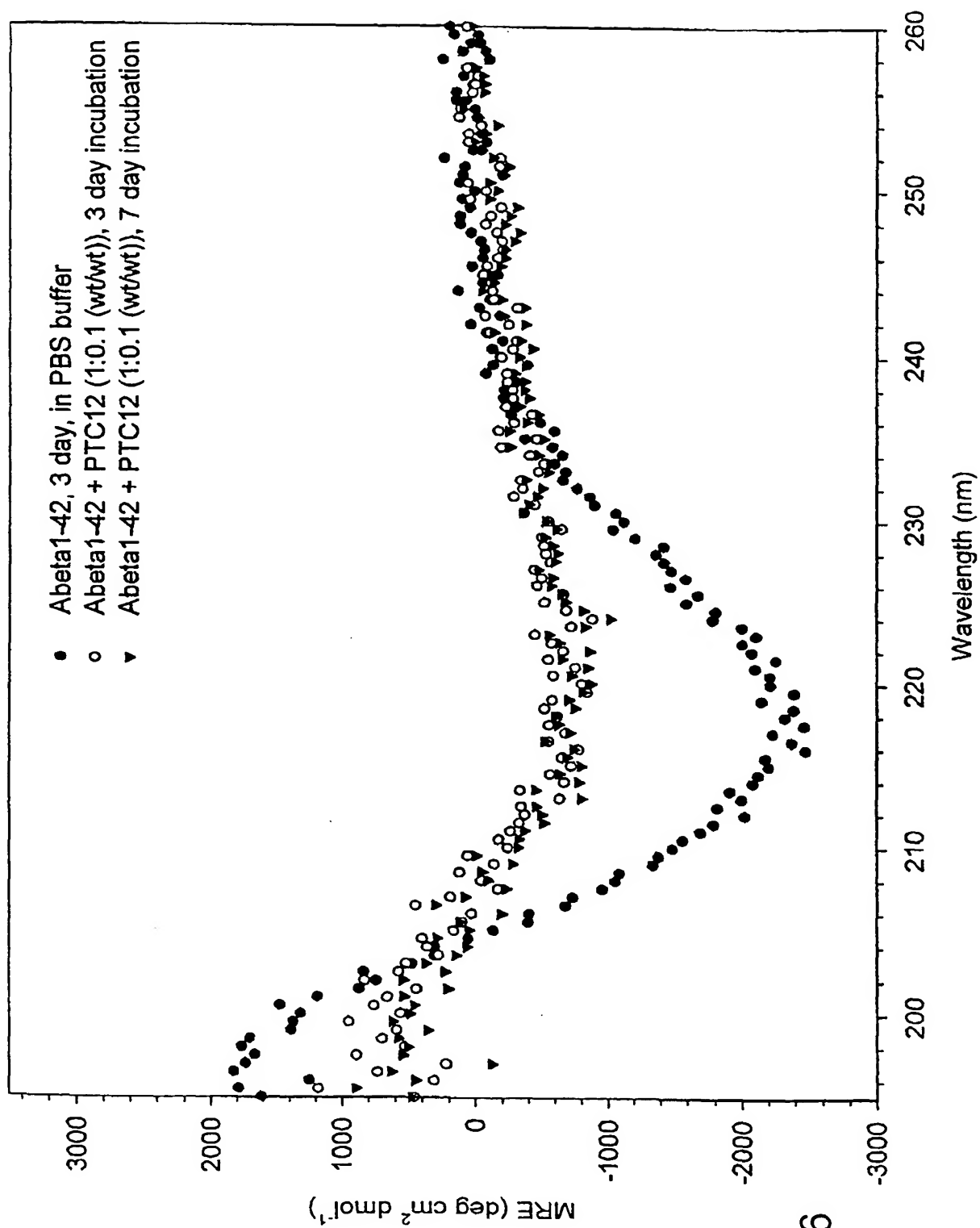


Fig. 6

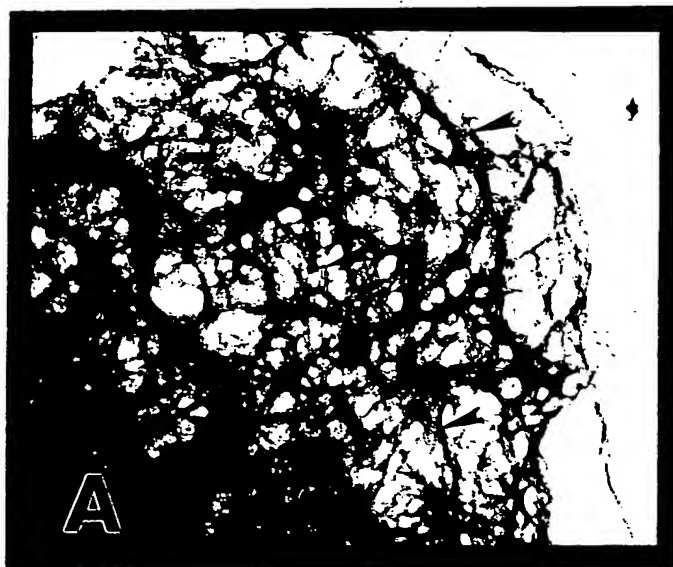


Fig. 7A

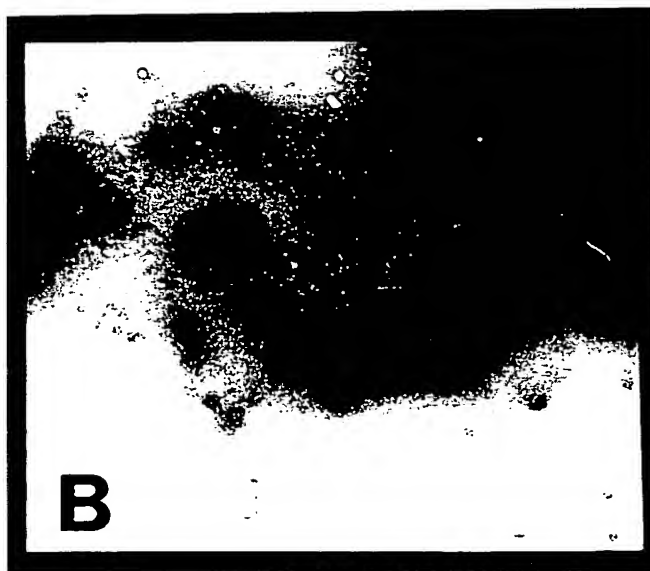


Fig. 7B



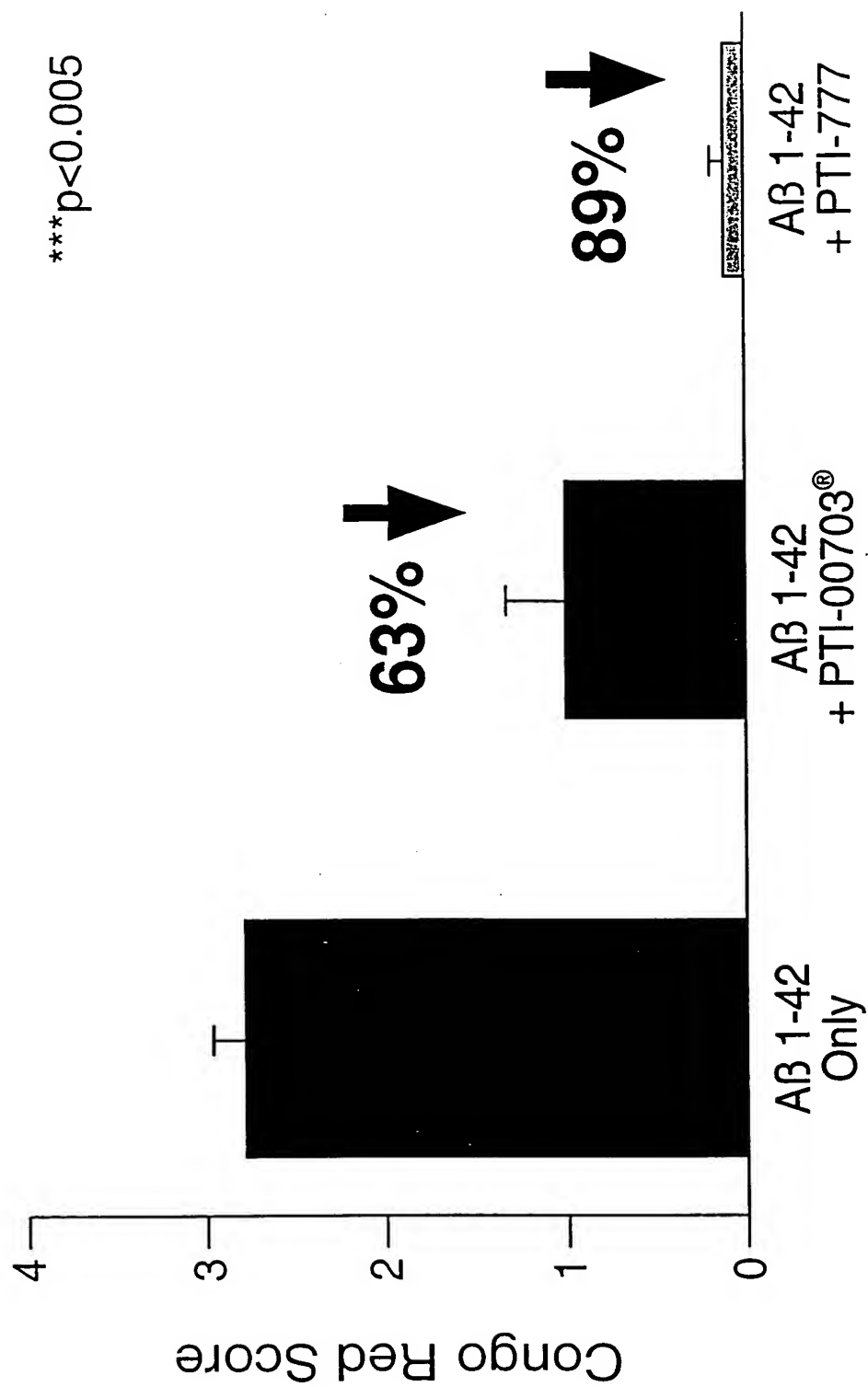


Fig. 8



Fig. 9A

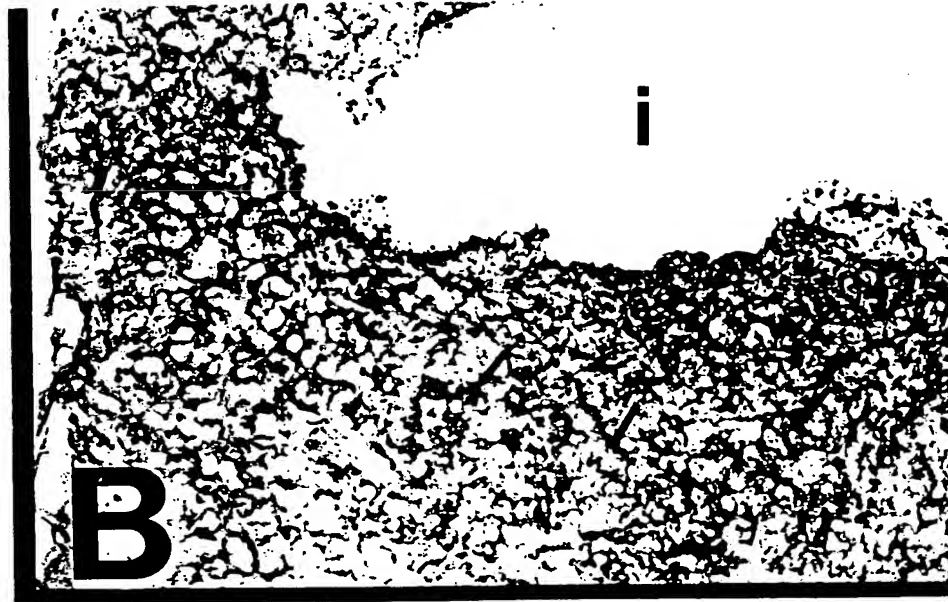


Fig. 9B



Fig. 9C



Fig. 9D

12/40

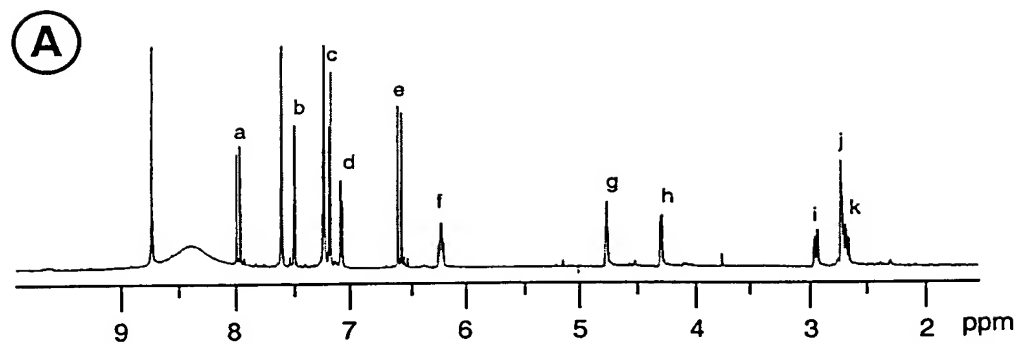


Fig. 10A

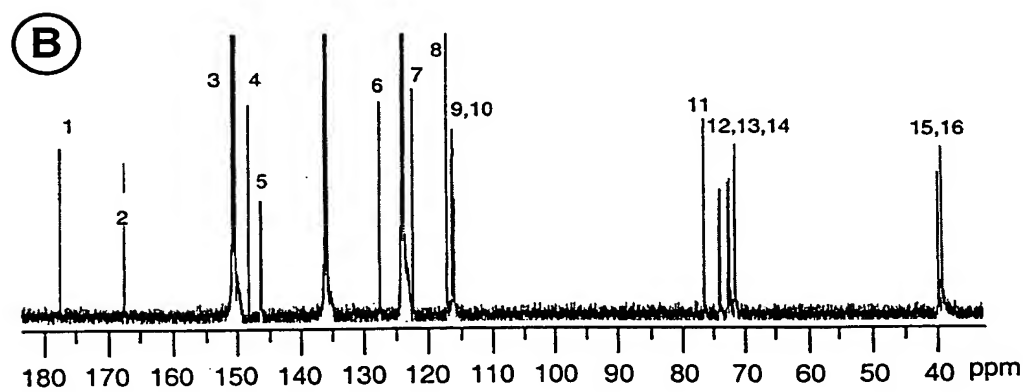


Fig.10B

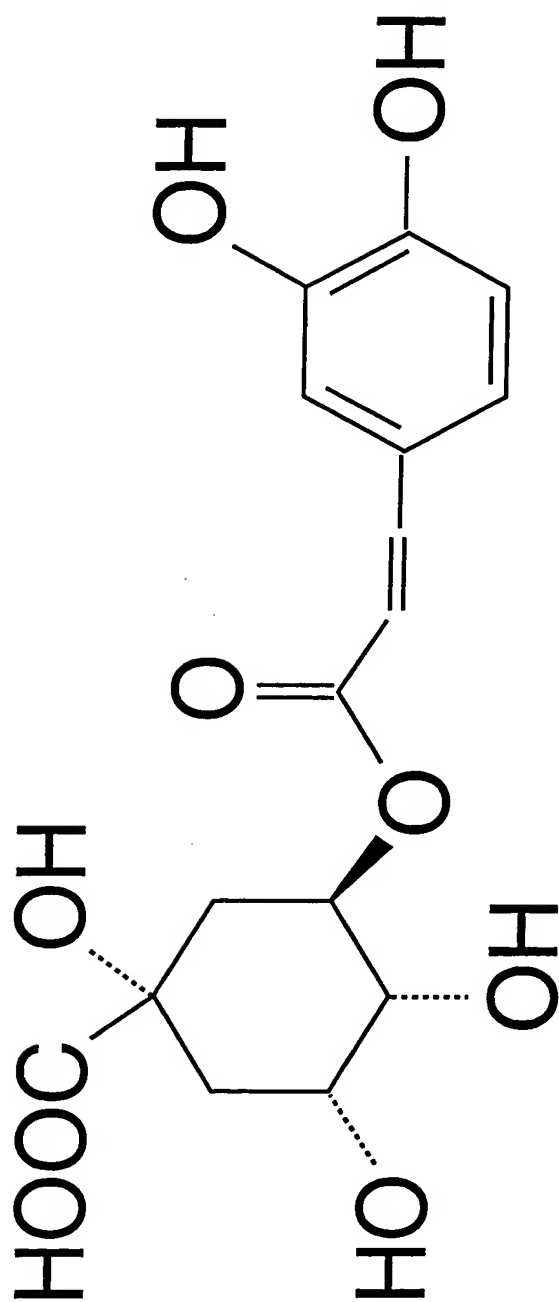


Fig. 11

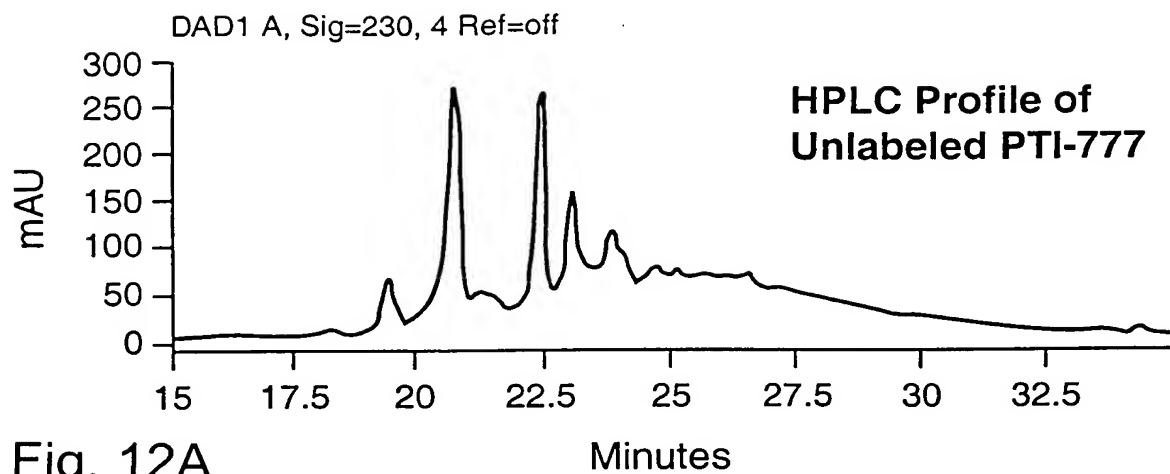


Fig. 12A

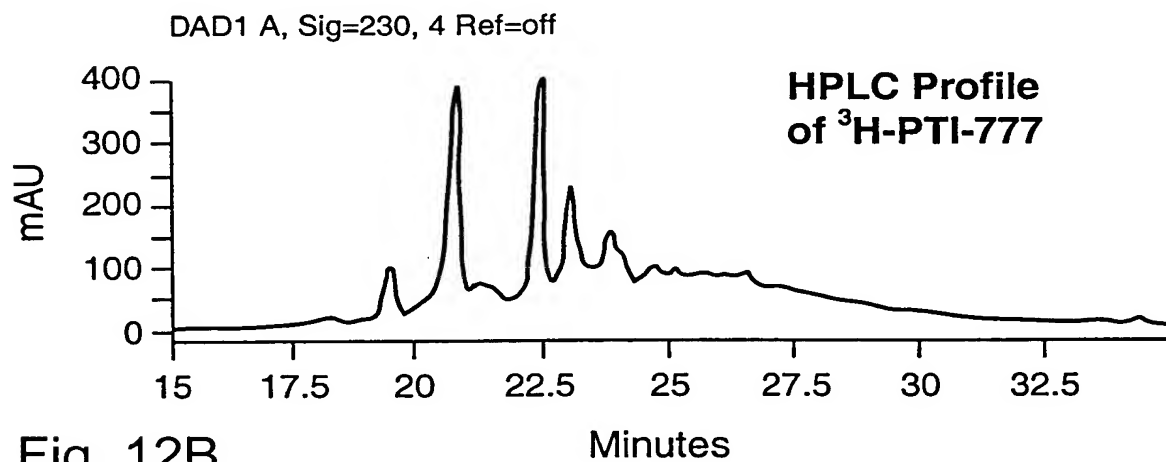


Fig. 12B

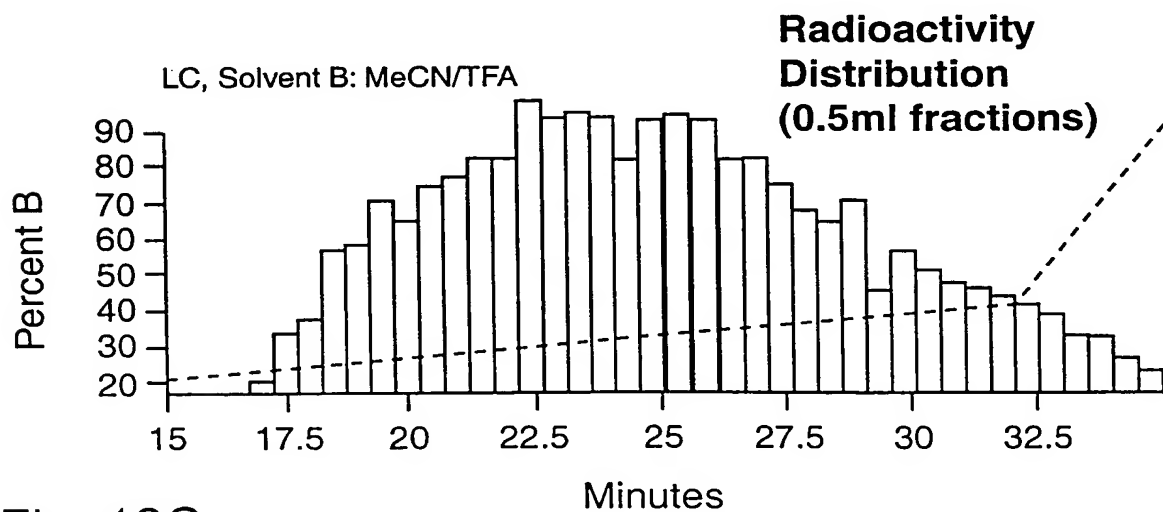


Fig. 12C

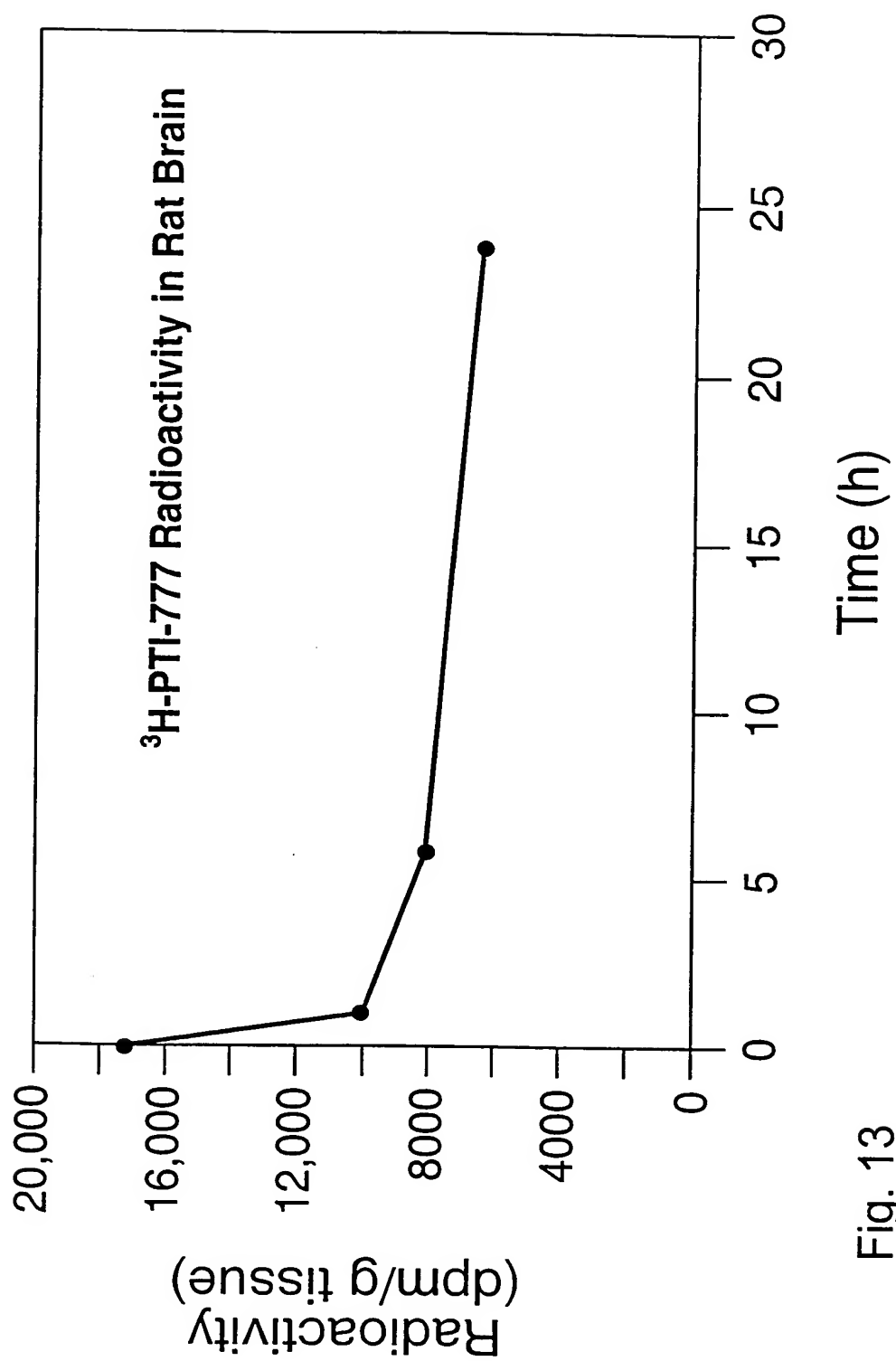


Fig. 13

16/40

# Jaguar Summed Mass Spectrum Report

File Name: G:\\_41.dat  
Method Name:  
Sample ID:  
Instrument: JAGUAR

Time Run: 11/13/00 11:01:40 AM  
Report Created: 11/13/00 11:03:26 AM  
Operator:  
Ionization Mode: ESI - positive ions

Spec # Range: 2706 - 2778

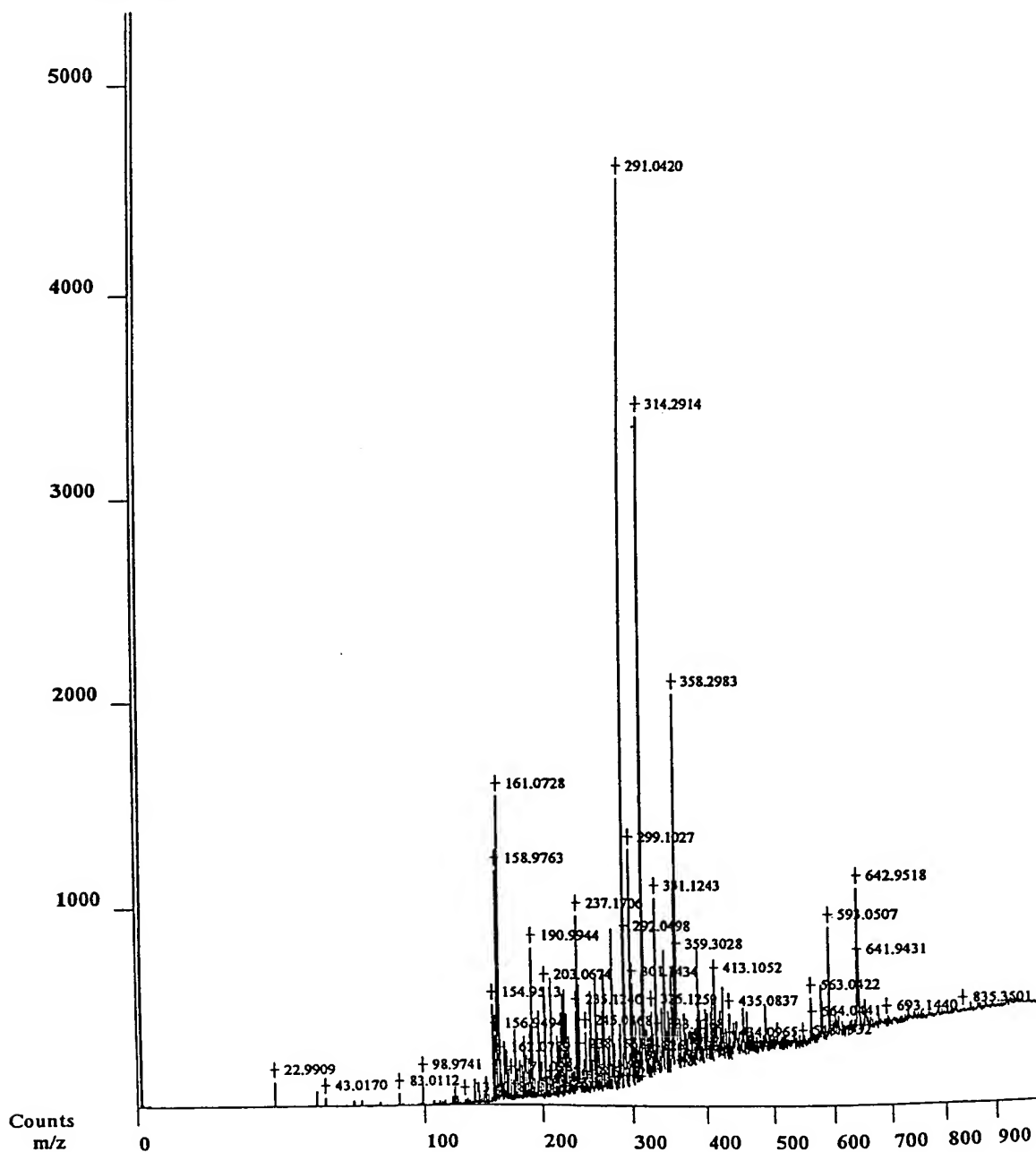


Fig. 14



17/40

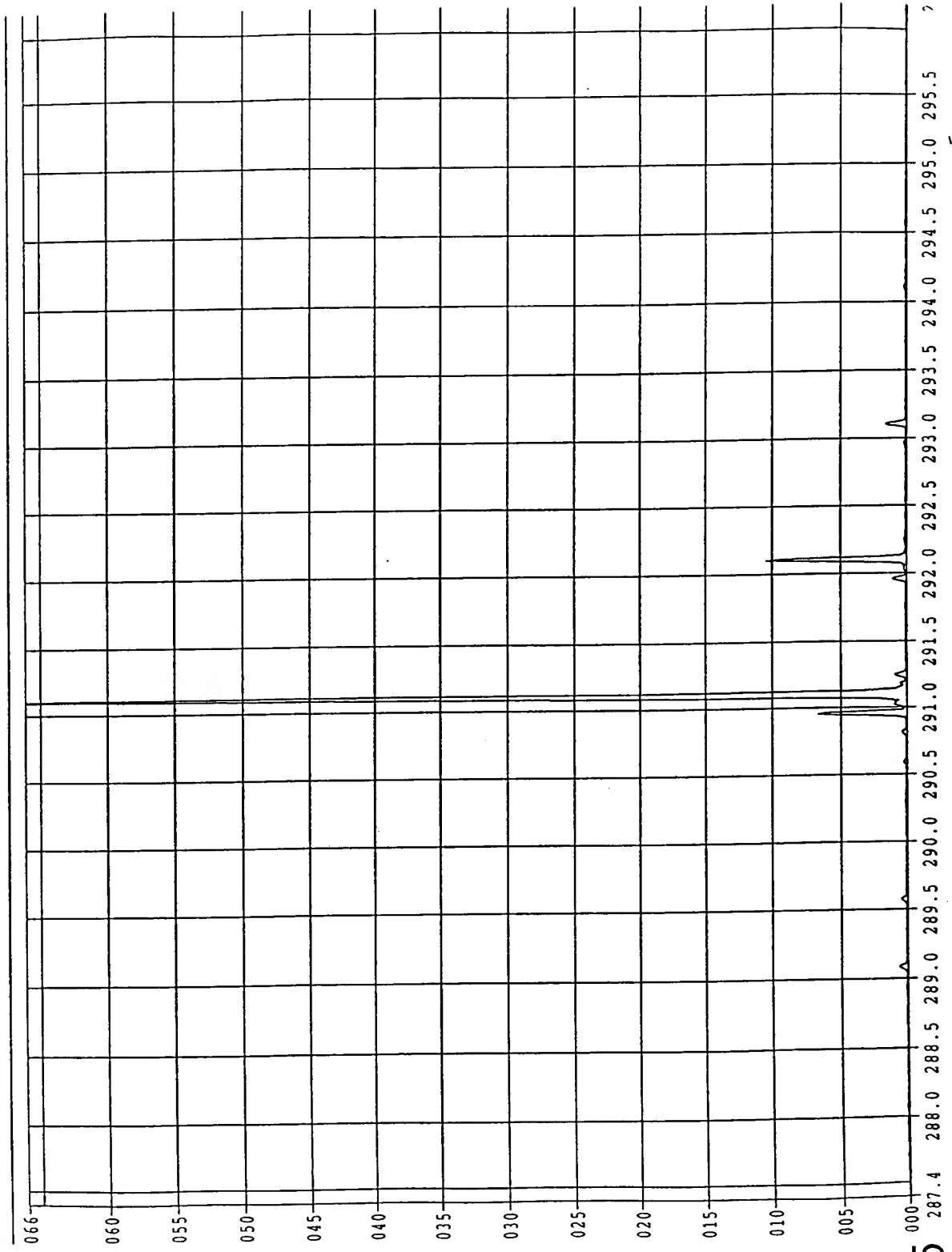


Fig. 15

18/40

( Mass Spectrum )  
Data : BYU\_A776  
Sample : I  
Note :  
Inlet : Direct Ion Mode : EI+  
Spectrum Type : Normal Ion (M<sup>+</sup>-Linear)  
RT : 0.64 min Scan# : (5,8)  
BP : m/z 140.0000 Int. : 135.19  
Output m/z range : 50.0000 to 362.6855 Cut Level : 0.00 %

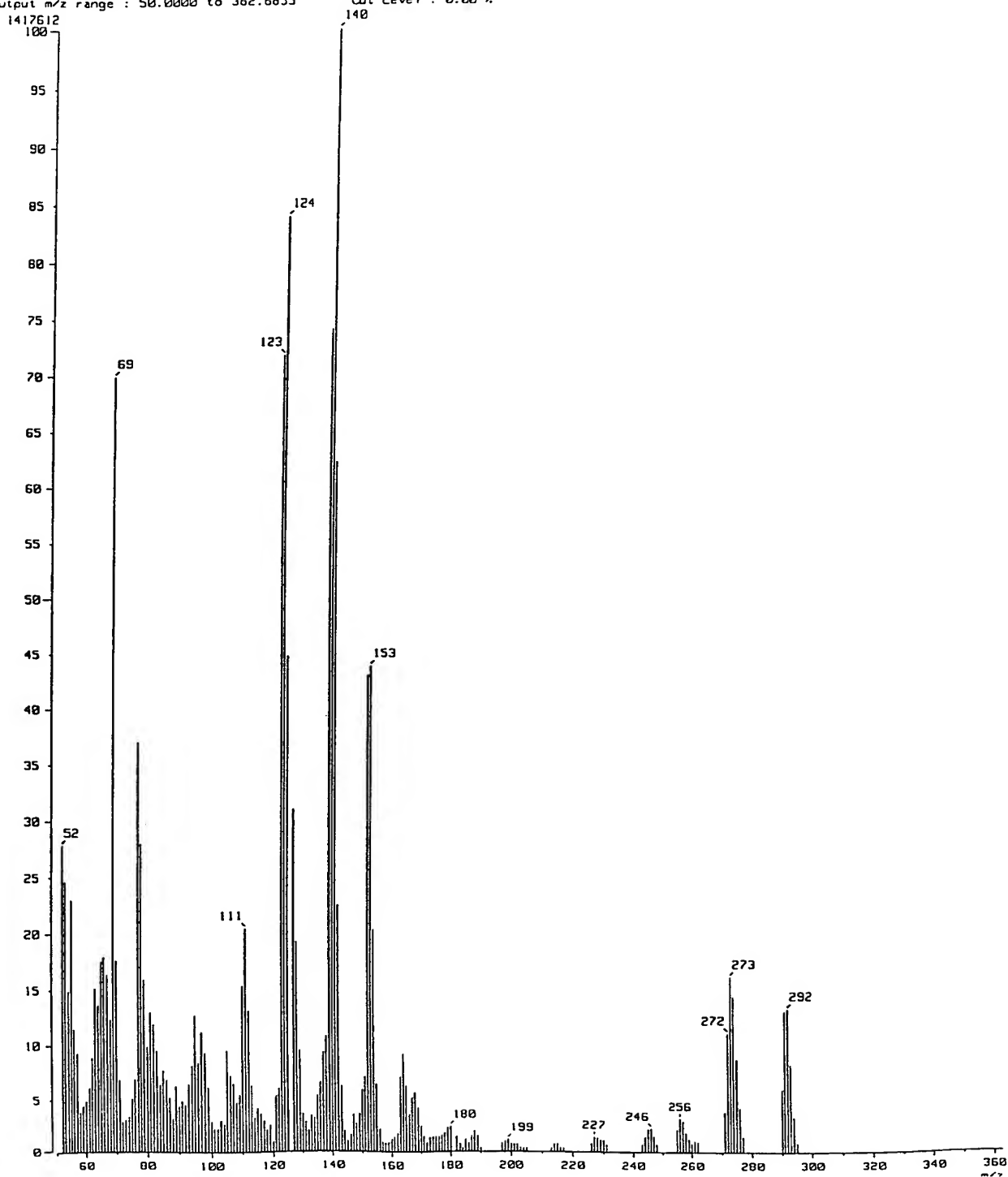


Fig. 16

19/40

( Mass Spectrum )  
Data : 0YU11349  
Sample: acylated I  
Note : thioGlycerol & Na  
Inlet : Direct Ion Mode : FAB+  
Spectrum Type : Normal Ion (MF-Linear)  
RT : 0.08 min Scan# : (1,4)  
BP : m/z 523.0000 Int. : 322.38  
Output m/z range : 240.0000 to 642.3739 Cut Level : 0.00 %  
3405255

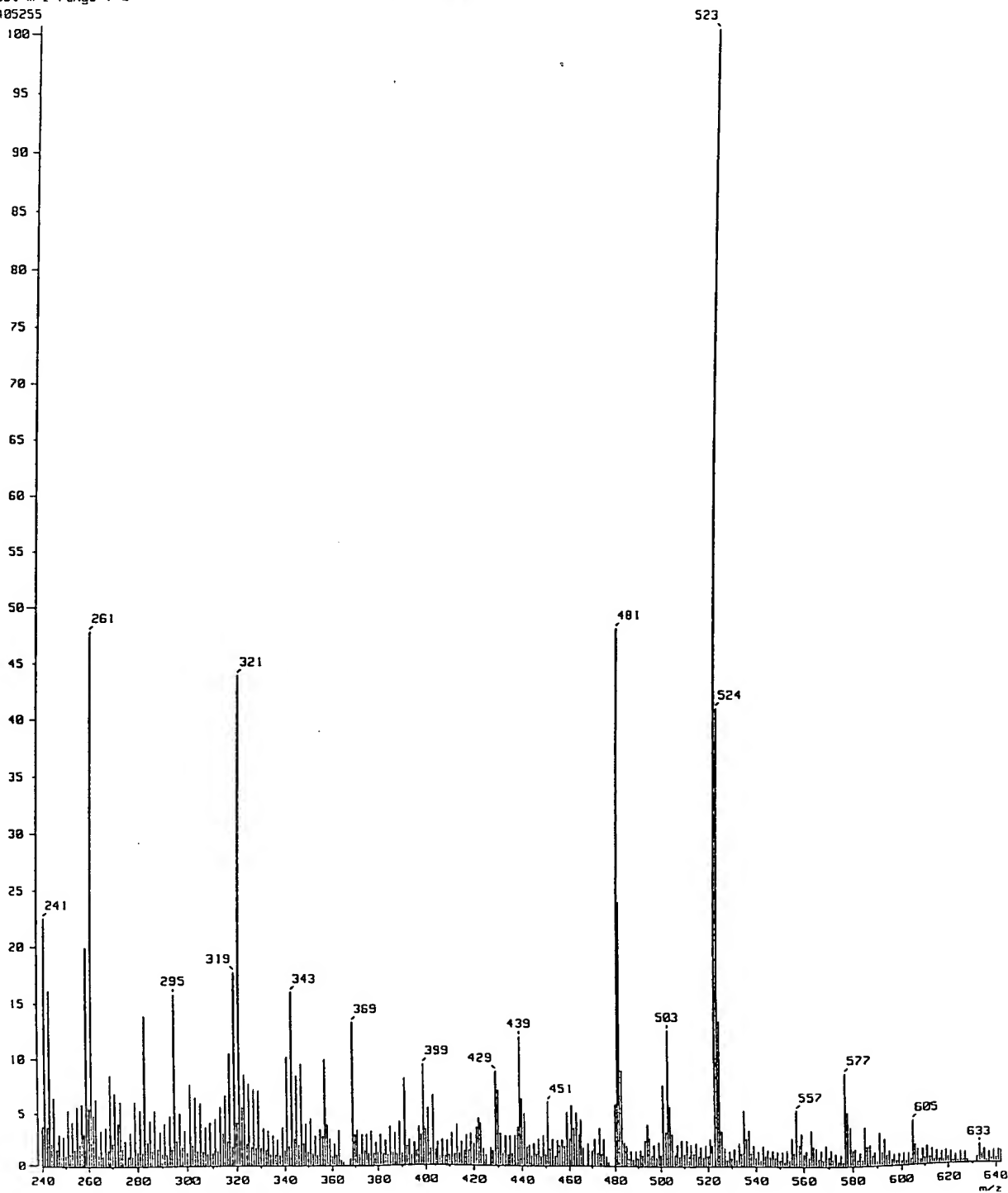


Fig. 17

20/40

[ Mass Spectrum ]  
Data : BYU 0373  
Sample: acylated-1  
Note :  
Inlet : Direct Ion Mode : EI+  
Spectrum Type : Normal Ion (HF-Linear)  
RT : 0.89 min Scan# : (7,9)-k((3,4))(k=1.0)  
BP : m/z 398.0000 Int. : 68.70  
Output m/z range : 50.0000 to 564.0950 Cut Level : 0.00 %

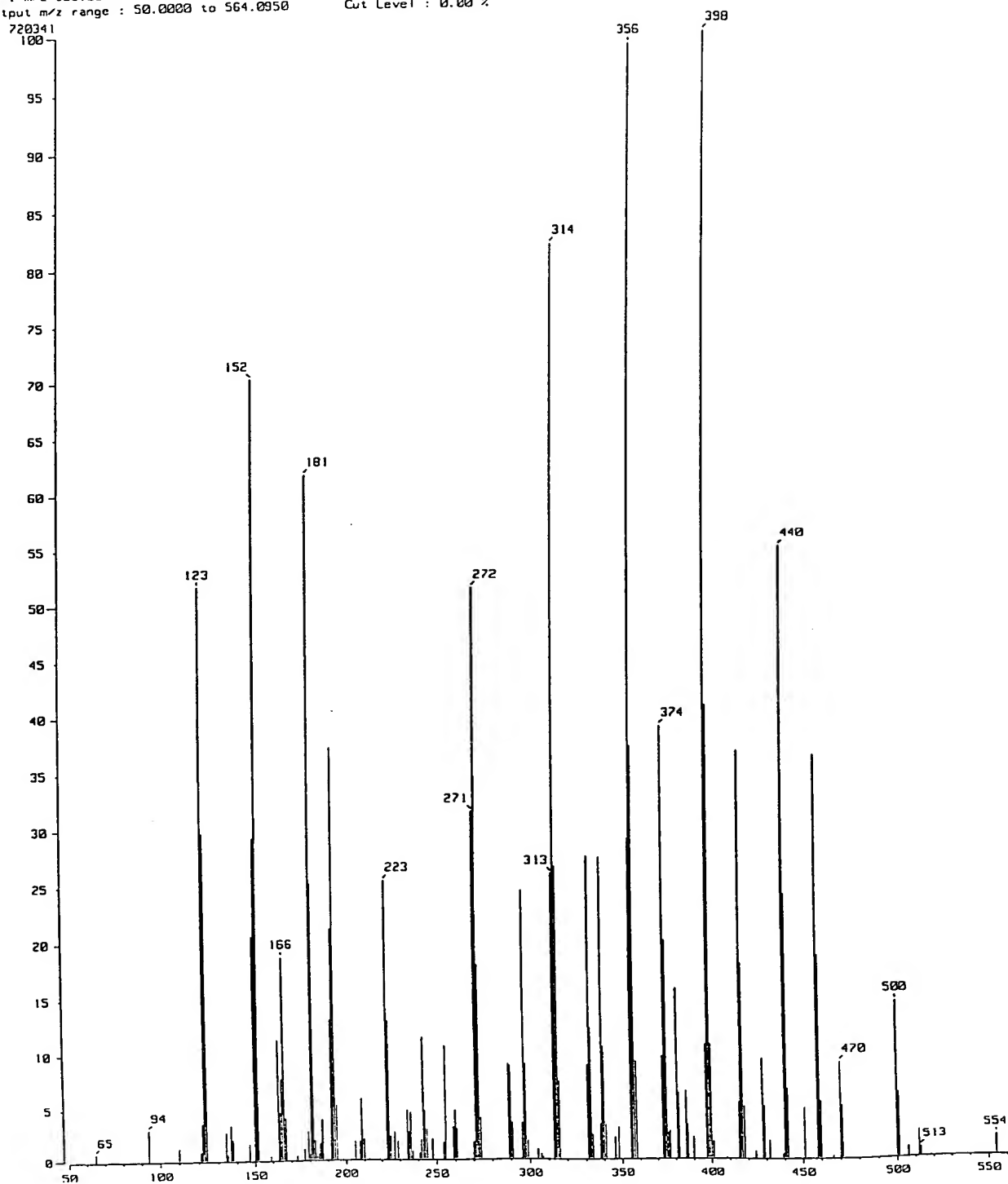


Fig. 18

H1 of sample

Pulse Sequence: s2pul

21/40

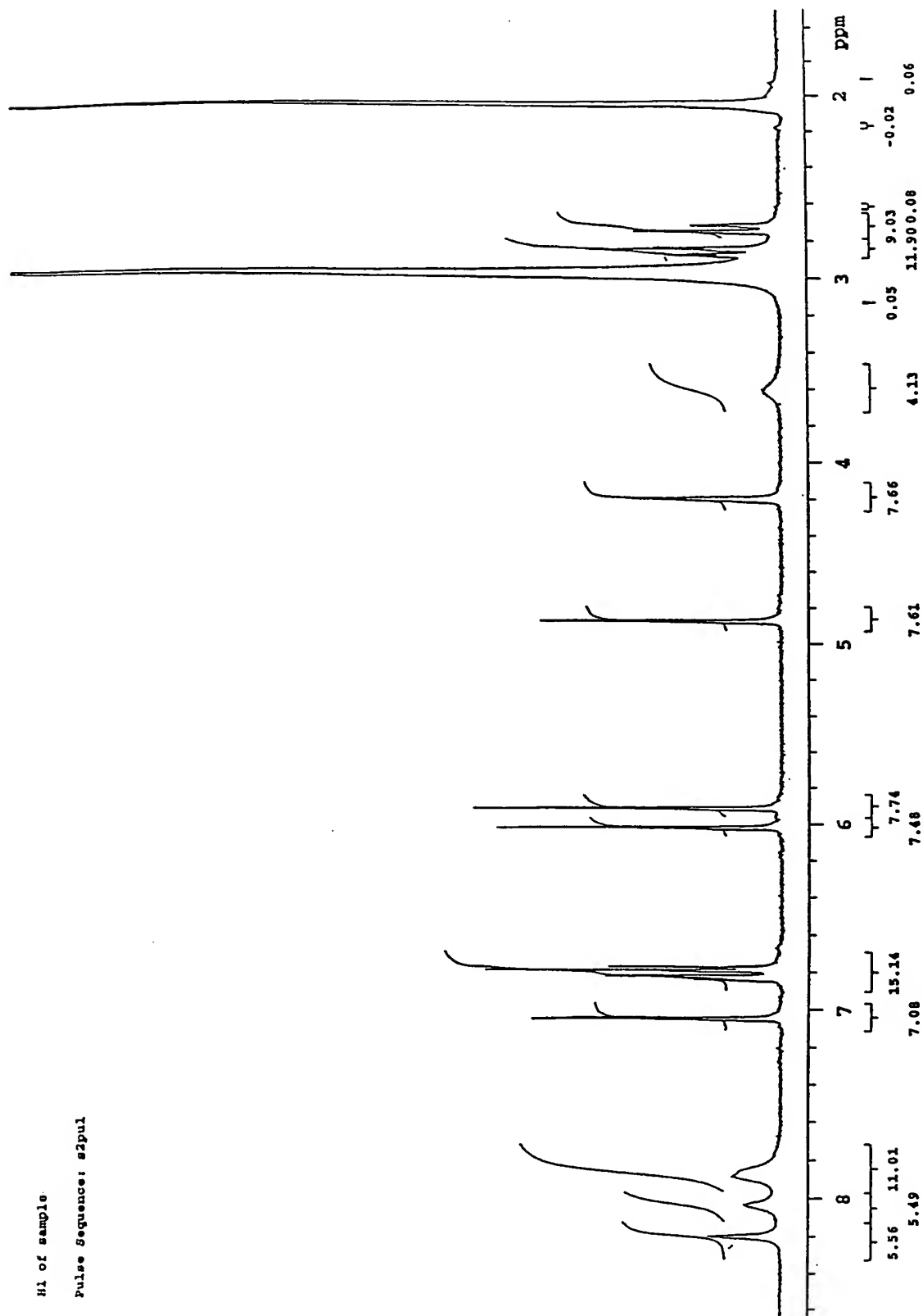


Fig. 19

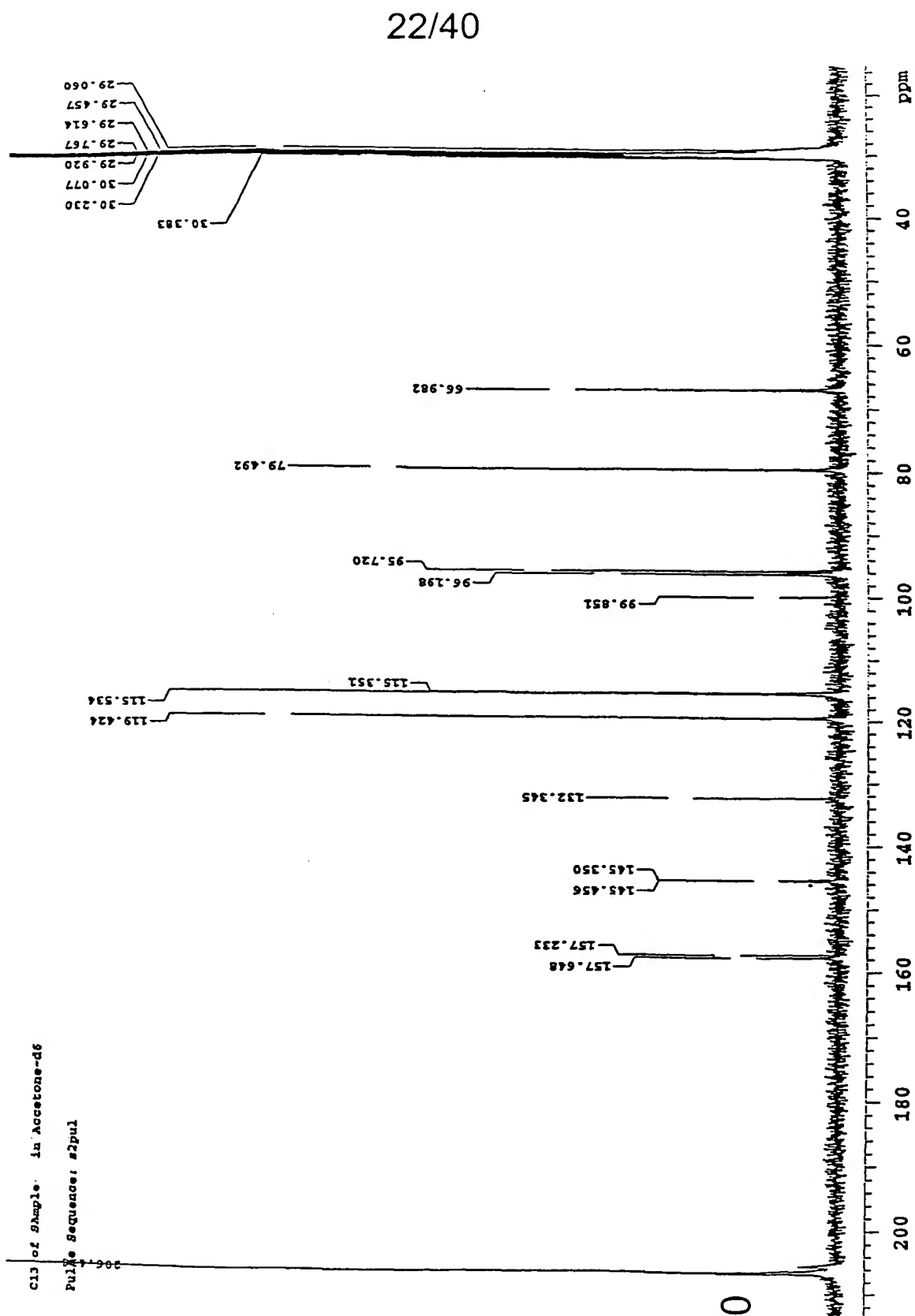


Fig. 20

H1

Pulse Sequence: s2pul

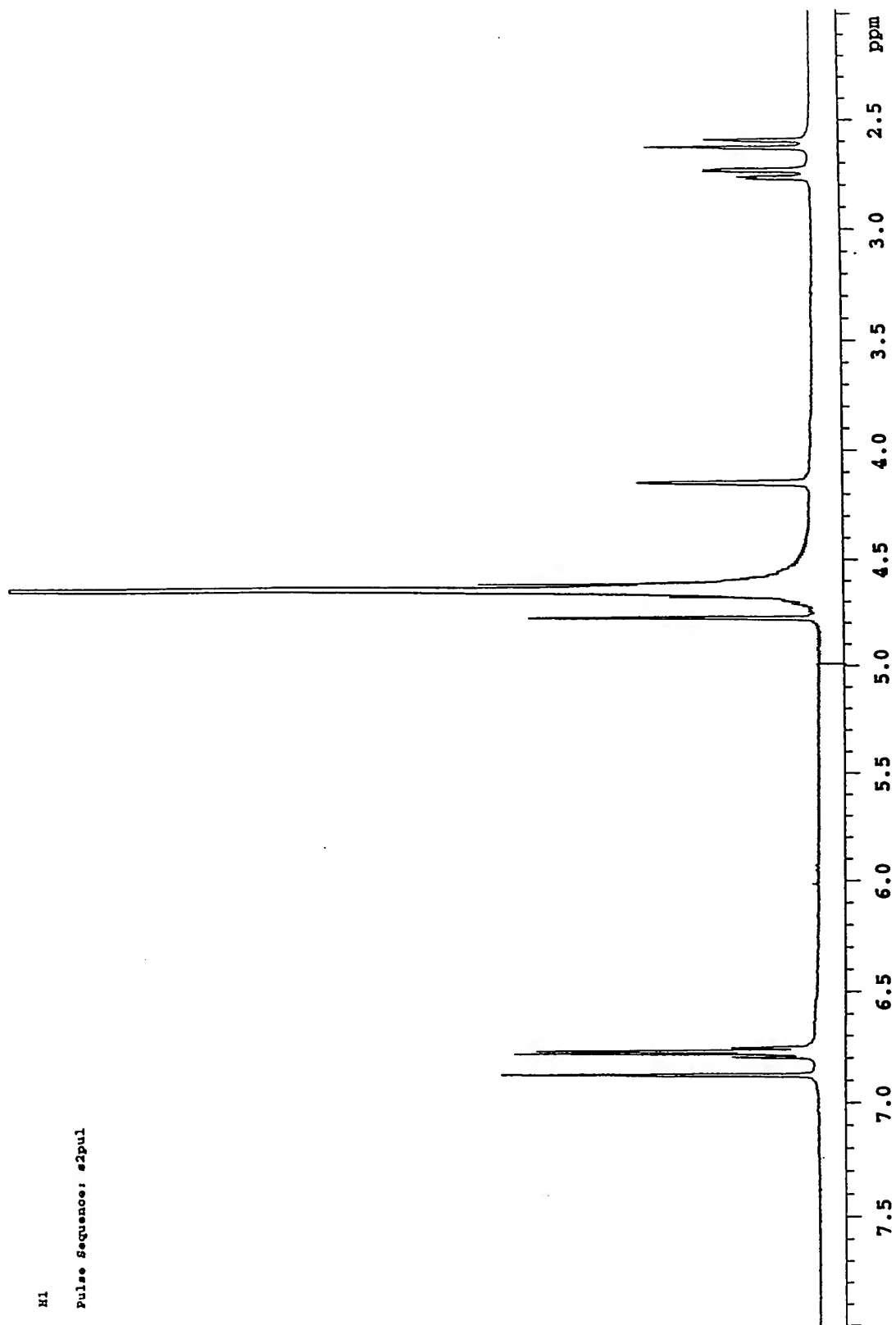


Fig. 21

C13 of Sample in D2O.

Pulse Sequence: s2pul

24/40

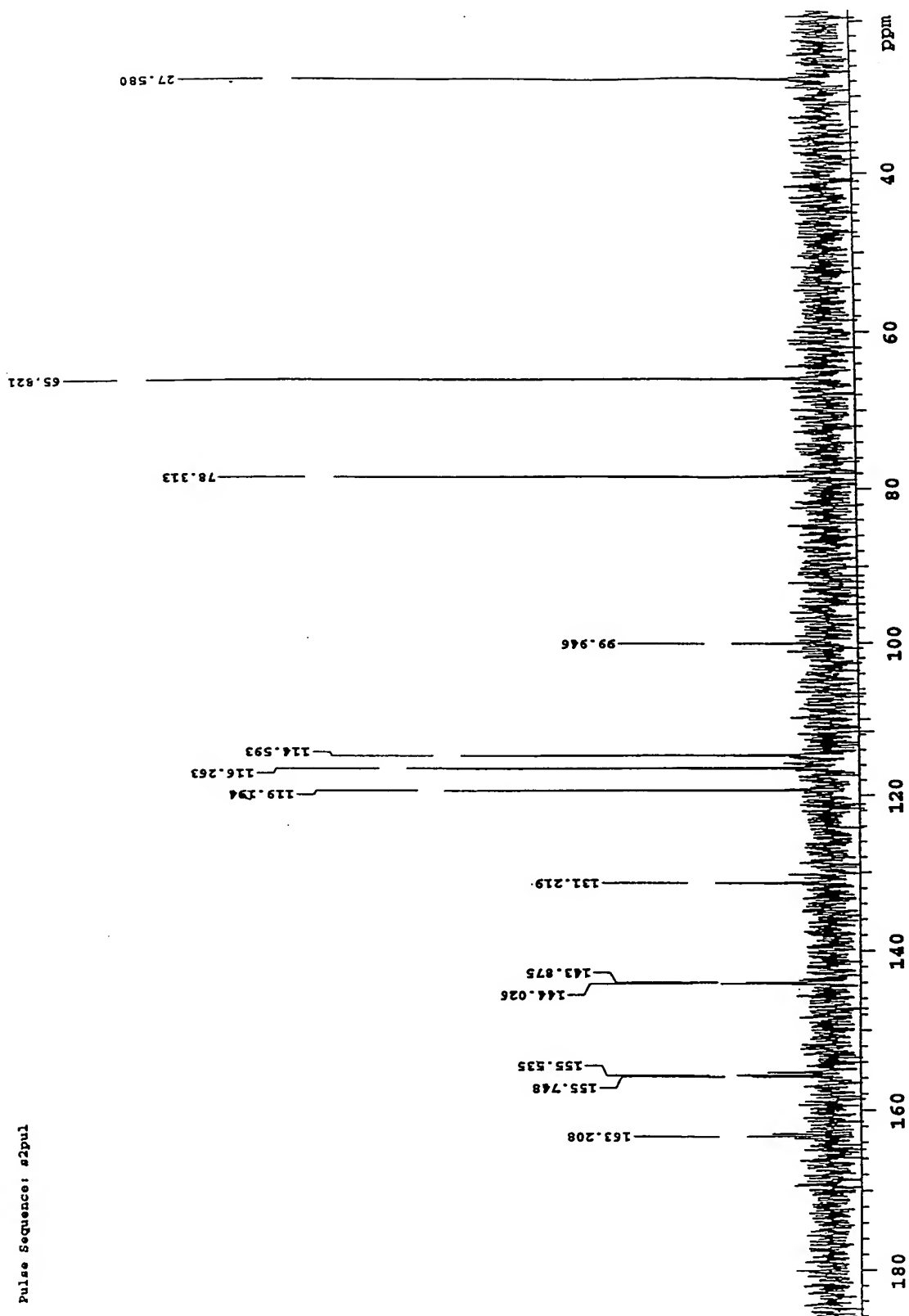
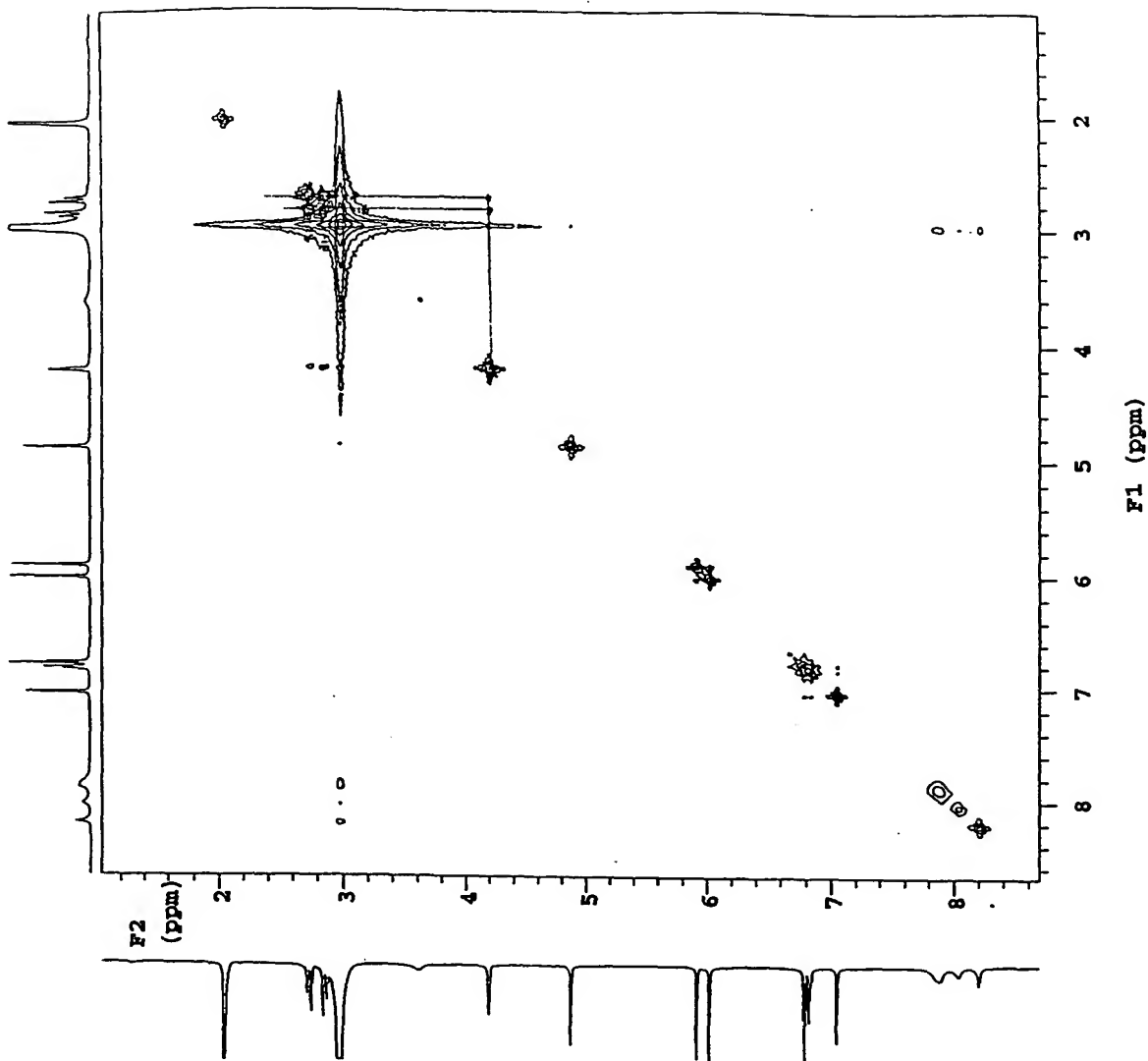


Fig. 22



25/40



COSY of Sample

Pulse Sequence: relayh

Solvent: Acetone

Ambient Temperature

UNITY-500 "nmr500"

PULSE SEQUENCE: relayh

COSY 90-90

Acq. time 0.302 sec

Width 3817.5 Hz

2D Width 3817.5 Hz

16 repetitions

159 increments

OBSERVE H1, 499.8814428 MHz

DATA PROCESSING

F1 DATA PROCESSING

Line broadening 0.3 Hz

PT size 1024 x 1024

Total time 16 min, 12 sec

Fig. 23

COSY

Pulse Sequence: relayh  
 Solvent: D2O  
 Ambient temperature  
 UNITY-500 "amx500"  
 PULSE SEQUENCE: relayh  
 Relax. delay 0.500 sec  
 COSY 90-90  
 Acq. time 0.178 sec  
 Width 2882.3 Hz  
 2D Width 2882.3 Hz  
 8 repetitions  
 120 increments  
 OBSERVE H1, 499.8801324 MHz  
 DATA PROCESSING  
 Line broadening 0.1 Hz  
 F1 DATA PROCESSING  
 Line broadening 0.3 Hz  
 FT size 1024 x 1024  
 Total time 11 min, 23 sec

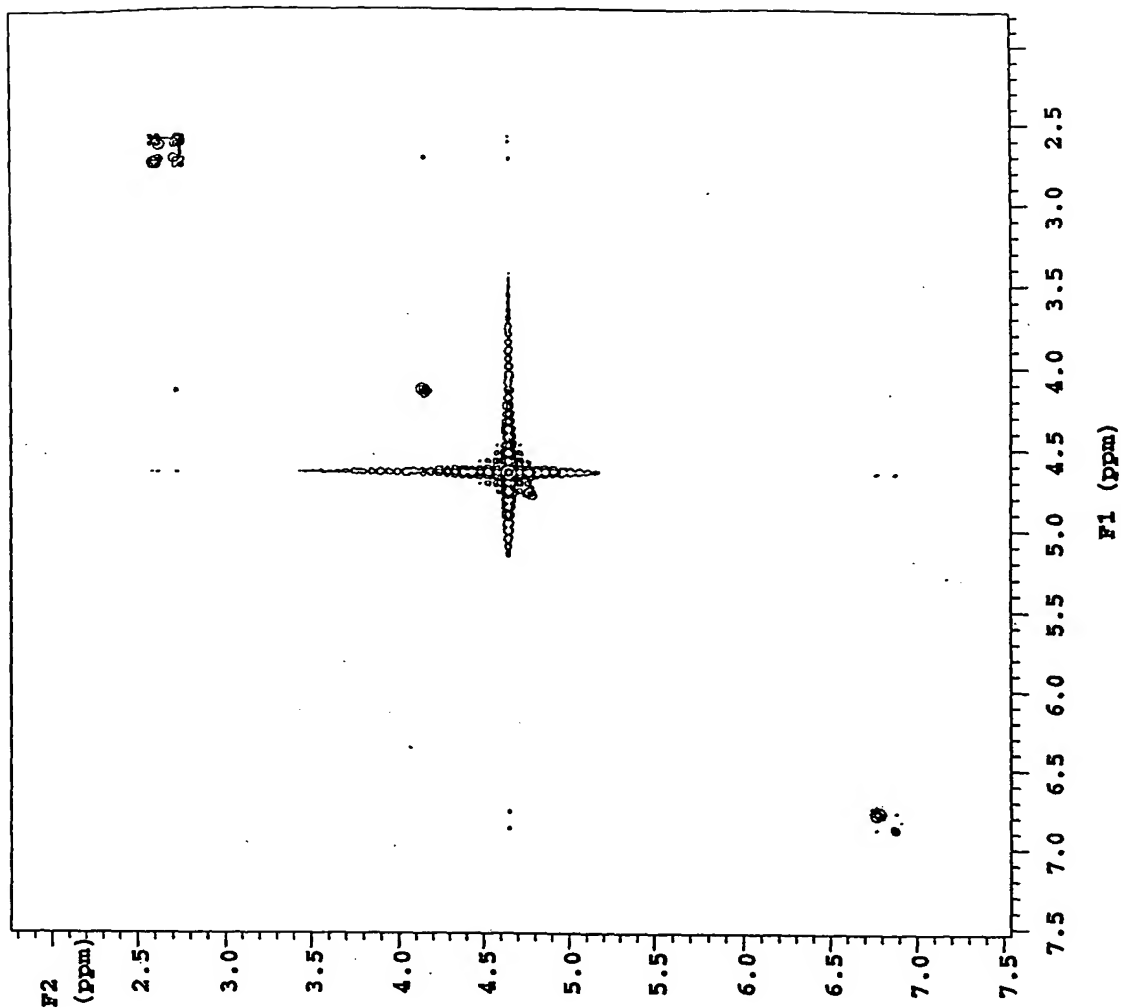
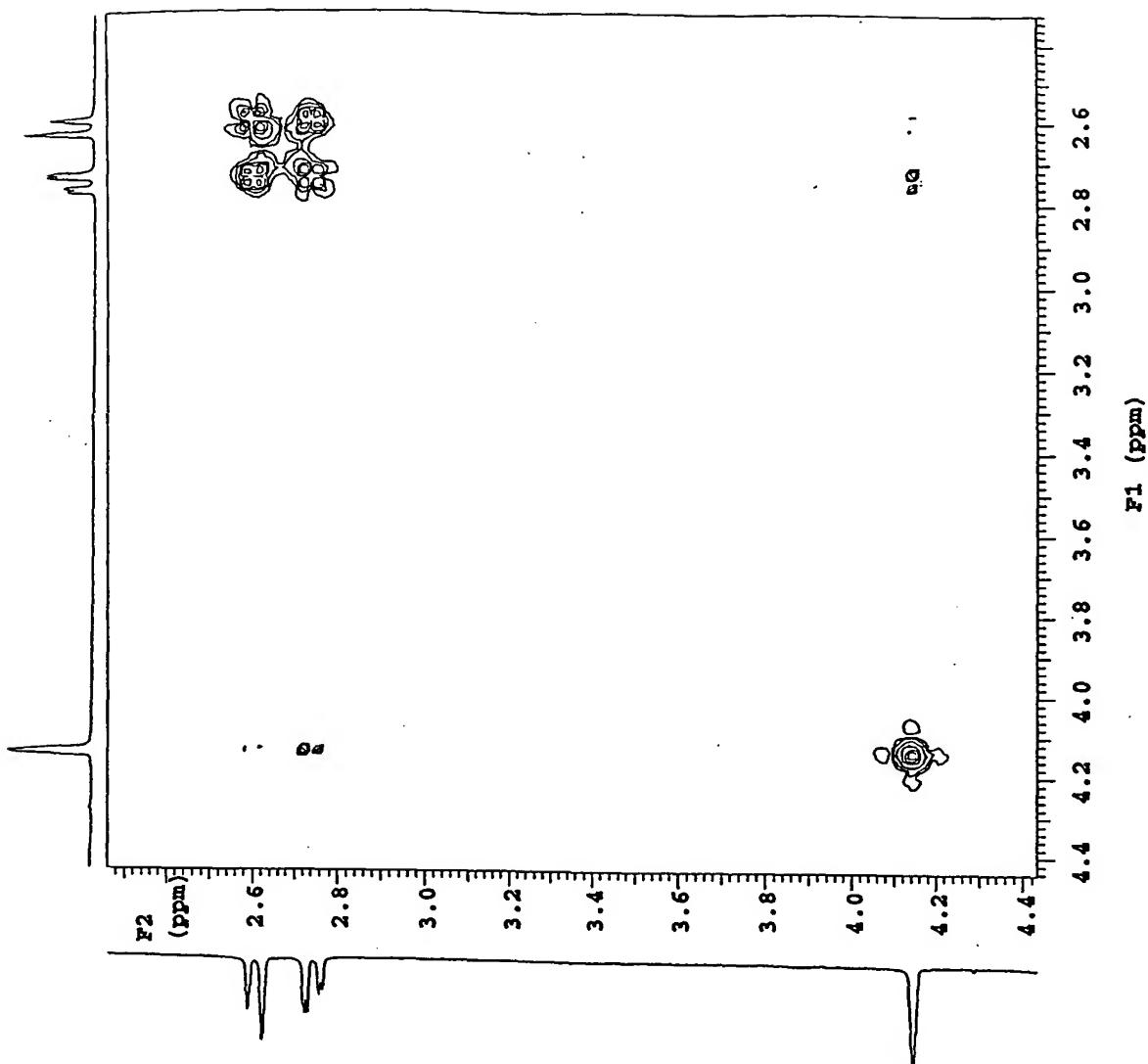


Fig. 24A



COSY

Pulse Sequence: relayh

Solvent: D2O

Ambient temperature

UNITY-500 "nmr500"

PULSE SEQUENCE: relayh

Relax. delay 0.500 sec

COSY 90-90

Acq. time 0.178 sec

Width 2882.3 Hz

2D Width 2882.3 Hz

8 repetitions

120 increments

OBSERVE H1, 499.8801324 MHz

DATA PROCESSING

Line broadening 0.1 Hz

F1 DATA PROCESSING

Line broadening 0.3 Hz

FT size 1024 x 1024

Total time 11 min, 23 sec

Fig. 24B

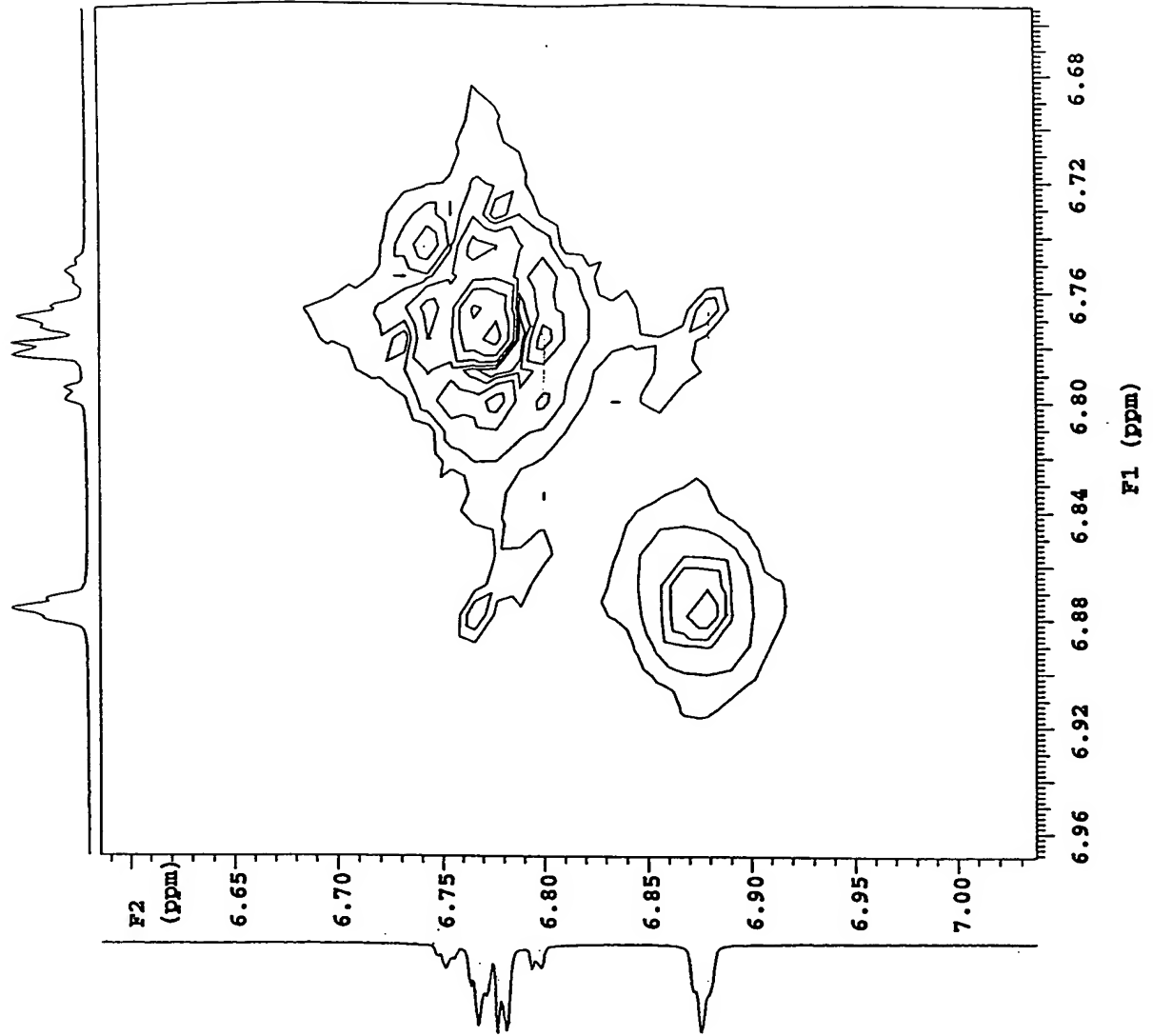


Fig. 24C

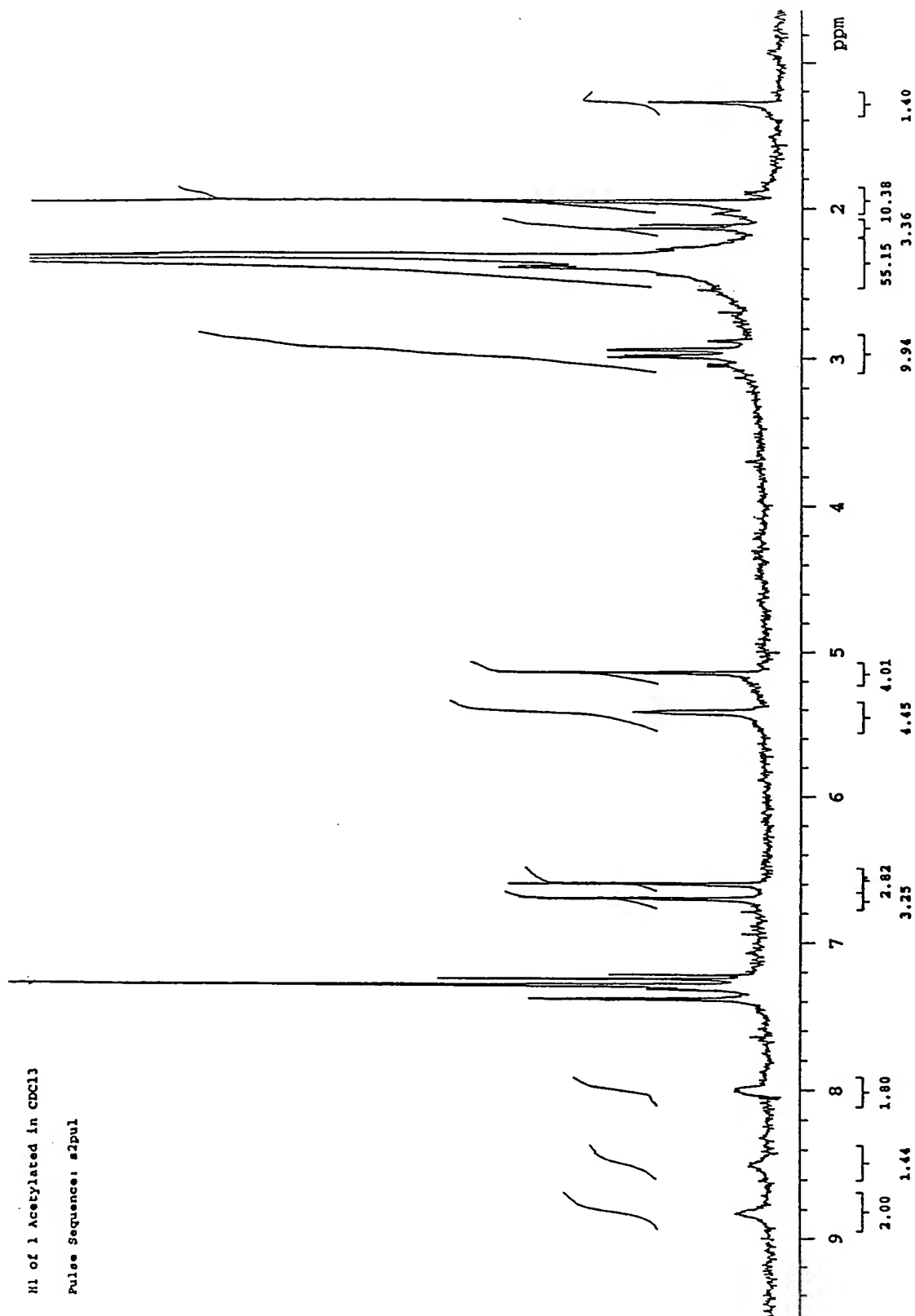
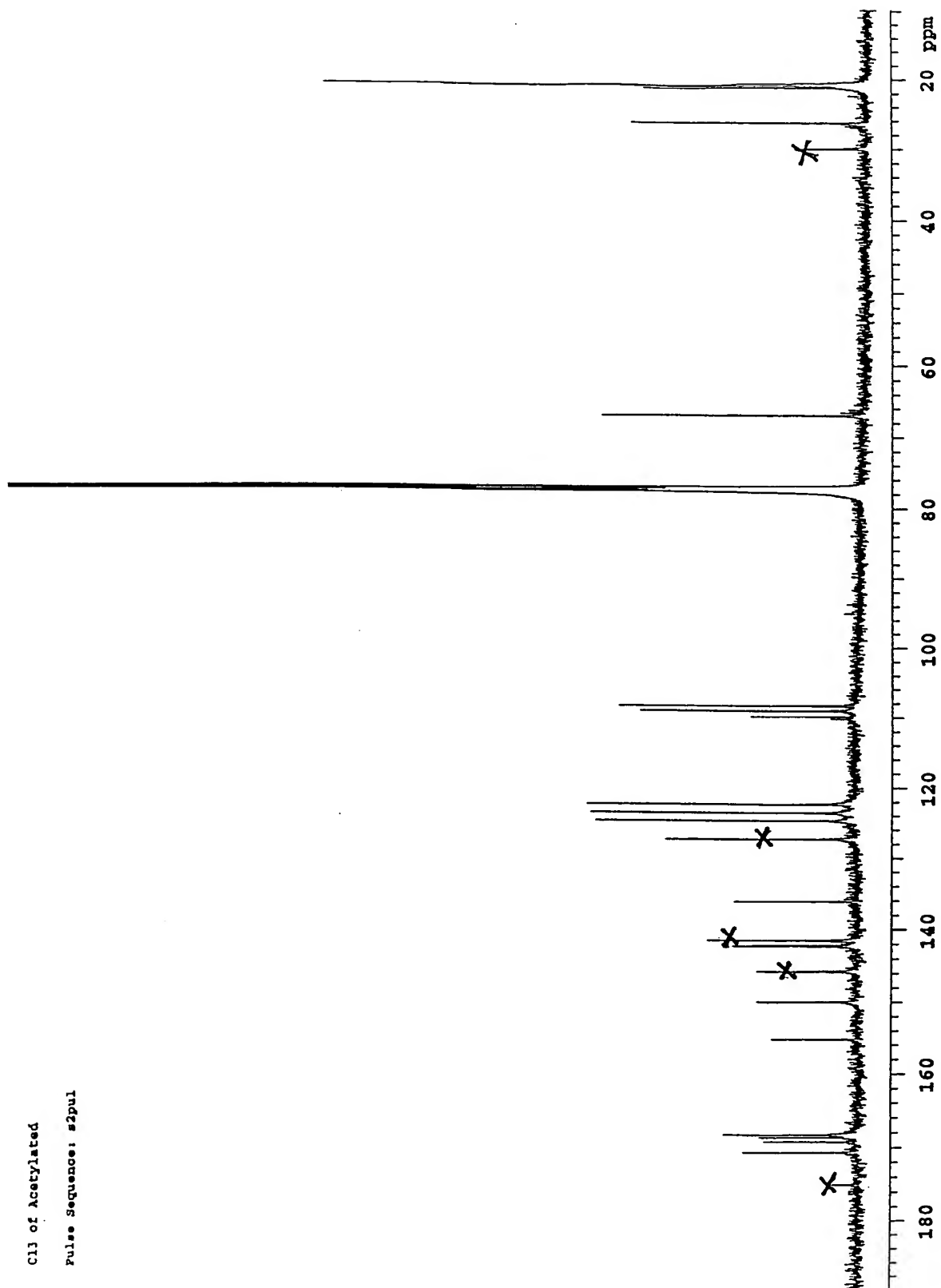


Fig. 25

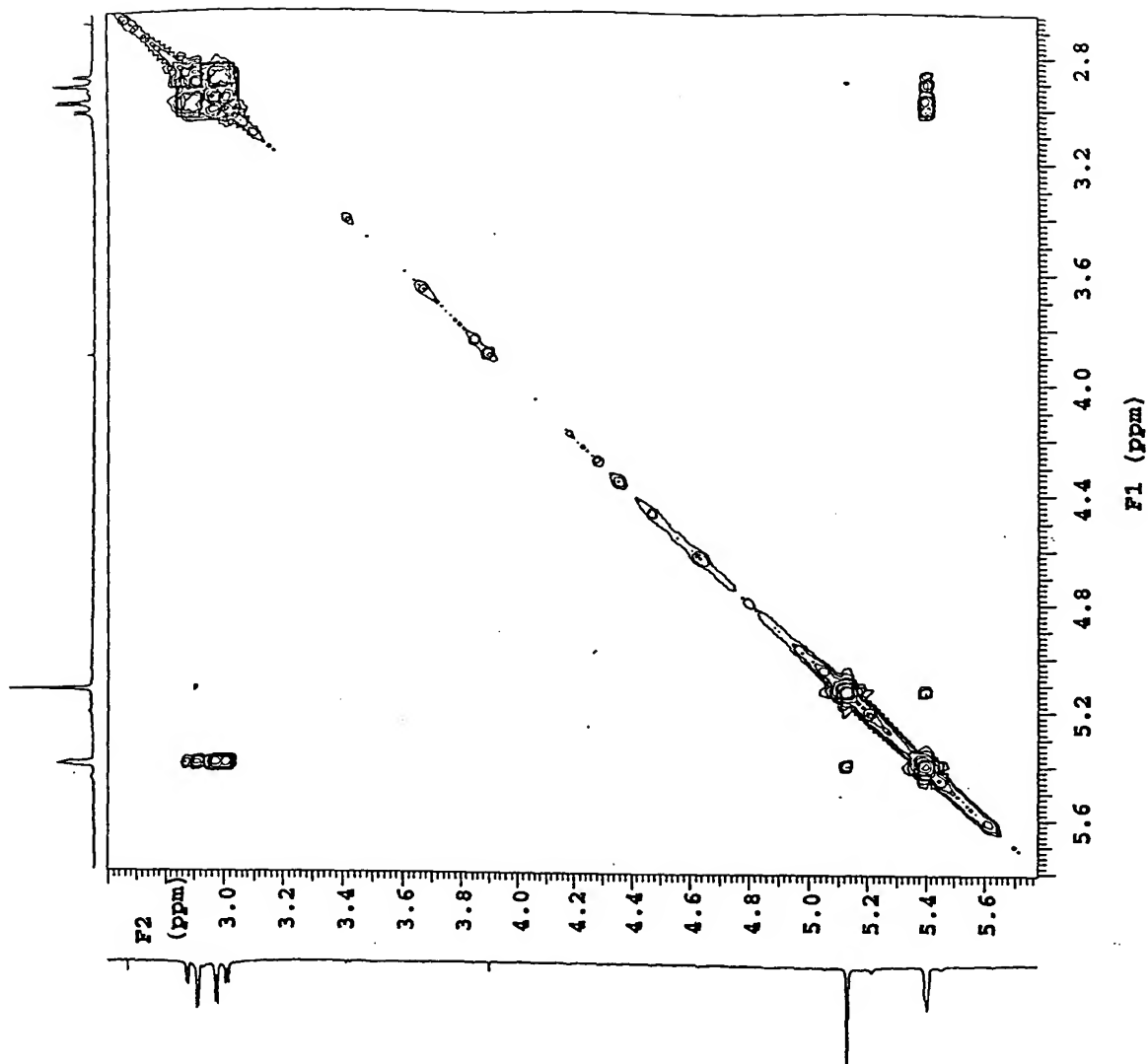
Cl3 of Acetylated  
Pulse Sequence: s2pul

30/40



X=pyridinium acetate

Fig. 26



COSY

Pulse Sequence: relayh

Solvent: CDCl3

Temp. 26.0 C / 299.1 K

INNOVA-500 "nmr500"

Relax. delay 0.500 sec

COSY 90-90

Acq. time 0.128 sec

Width 8000.0 Hz

2D Width 8000.0 Hz

16 repetitions

512 increments

OBSERVE H1, 499.9135718 MHz

DATA PROCESSING

Sine bell 0.064 sec

F1 DATA PROCESSING

Sine bell 0.032 sec

FT size 2048 x 2048

Total time 1 hr, 31 min, 32 sec

Fig. 27

HETCOR of Acetylated . in CDCl<sub>3</sub>.

Pulse Sequence: hetcor

Solvent: CDCl<sub>3</sub>

Temp. 26.0 C / 299.1 K

User: 1-14-87

INOVA-500 "nmr500"

Relax. delay 1.000 sec

Acq. time 0.082 sec

Width 25000.0 Hz

2D Width 4614.9 Hz

208 repetitions

256 increments

OBSERVE C13, 125.7033376 MHz

DECOUPLE H1, 499.9160715 MHz

Power 38 dB

on during acquisition

off during delay

WALTZ-16 modulated

DATA PROCESSING

Line broadening 2.0 Hz

F1 DATA PROCESSING

Line broadening 0.3 Hz

FT size 4096 x 1024

Total time 16 hr, 46 min, 21 sec

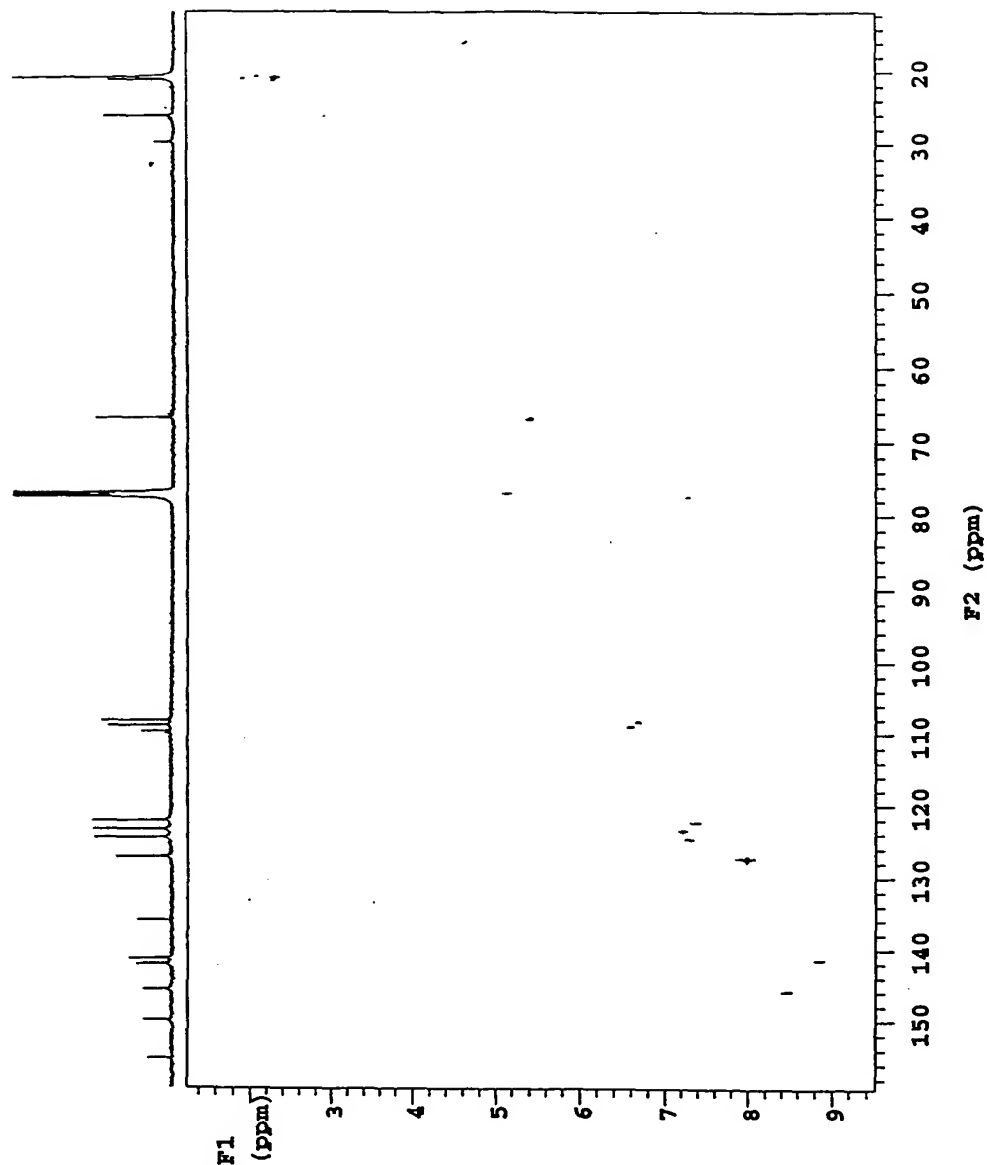


Fig. 28A



HETCOR of Acetylated in CDCl<sub>3</sub>.

X=pyridinium acetate

Pulse Sequence: hetcor

Solvent: CDCl<sub>3</sub>

Temp. 26.0 C / 299.1 K

User: I-14-87

INOVA-500 "mar500"

Relax. delay 1.000 sec

Acq. time 0.082 sec

Width 25000.0 Hz

2D Width 4614.9 Hz

208 repetitions

256 increments

OBSERVE C13, 125.703376 MHz

DECOUPLE H1, 499.9160715 MHz

Power 38 dB

on during acquisition

off during delay

WALTZ-16 modulated

DATA PROCESSING

Line broadening 2.0 Hz

F1 DATA PROCESSING

Line broadening 0.3 Hz

FT size 4096 x 1024

Total time 16 hr, 46 min, 21 sec

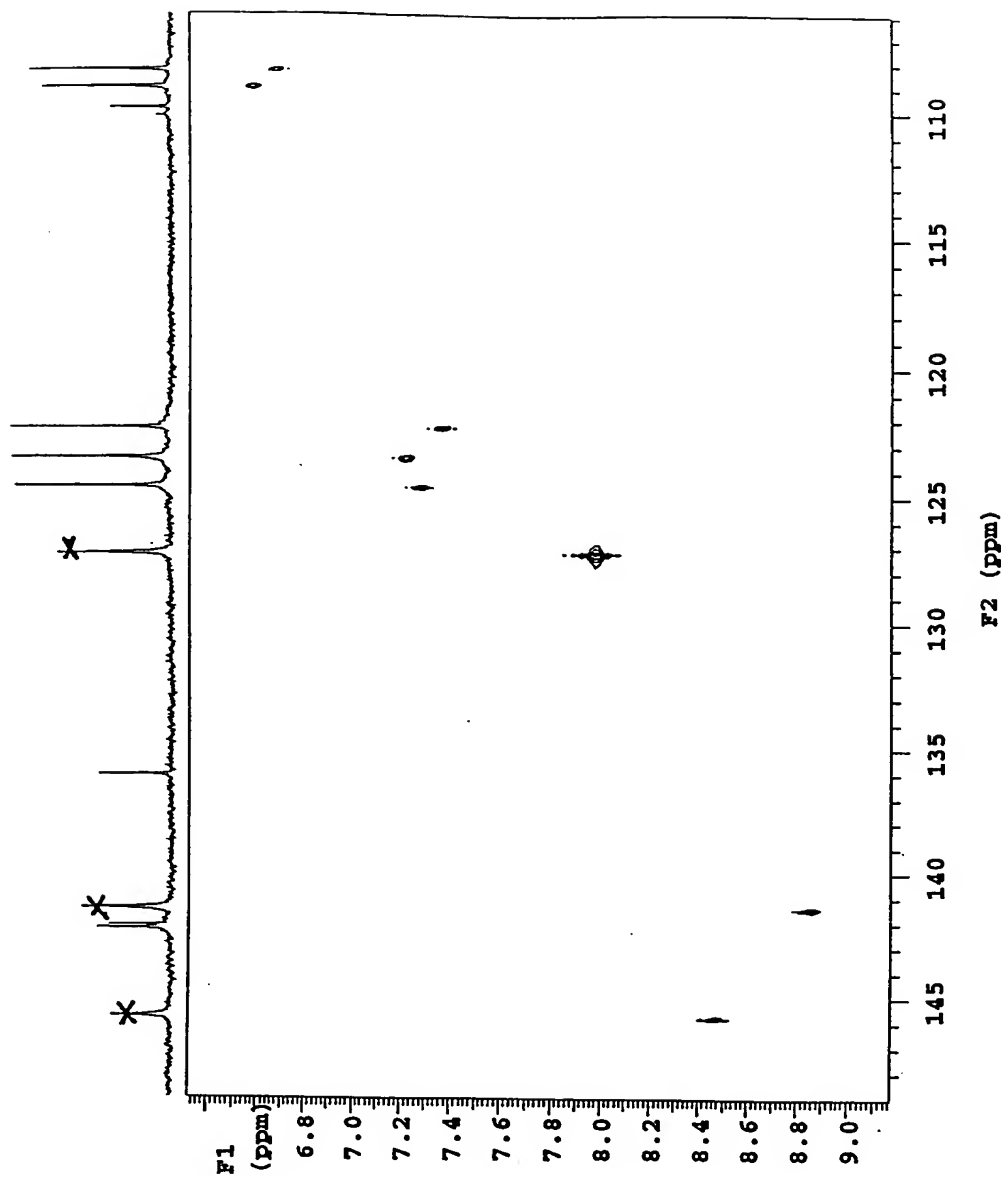


Fig. 28B

HETCOR of Acetylated in CDCl<sub>3</sub>.

Pulse Sequence: hetcor

Solvent: CDCl<sub>3</sub>

Temp. 26.0 C / 299.1 K

User: 1-14-87

INOVA-500 "nmr500"

Relax. delay 1.000 sec

Acq. time 0.082 sec

Width 25000.0 Hz

2D Width 4614.9 Hz

208 repetitions

256 increments

OBSERVE C13, 125.7033376 MHz

DECOUPLE H1, 499.9160715 MHz

Power 38 dB

on during acquisition

off during delay

WALTZ-16 modulated

DATA PROCESSING

Line broadening 2.0 Hz

F1 DATA PROCESSING

Line broadening 0.3 Hz

FT size 4096 x 1024

Total time 16 hr, 46 min, 21 sec

X=pyridinium acetate

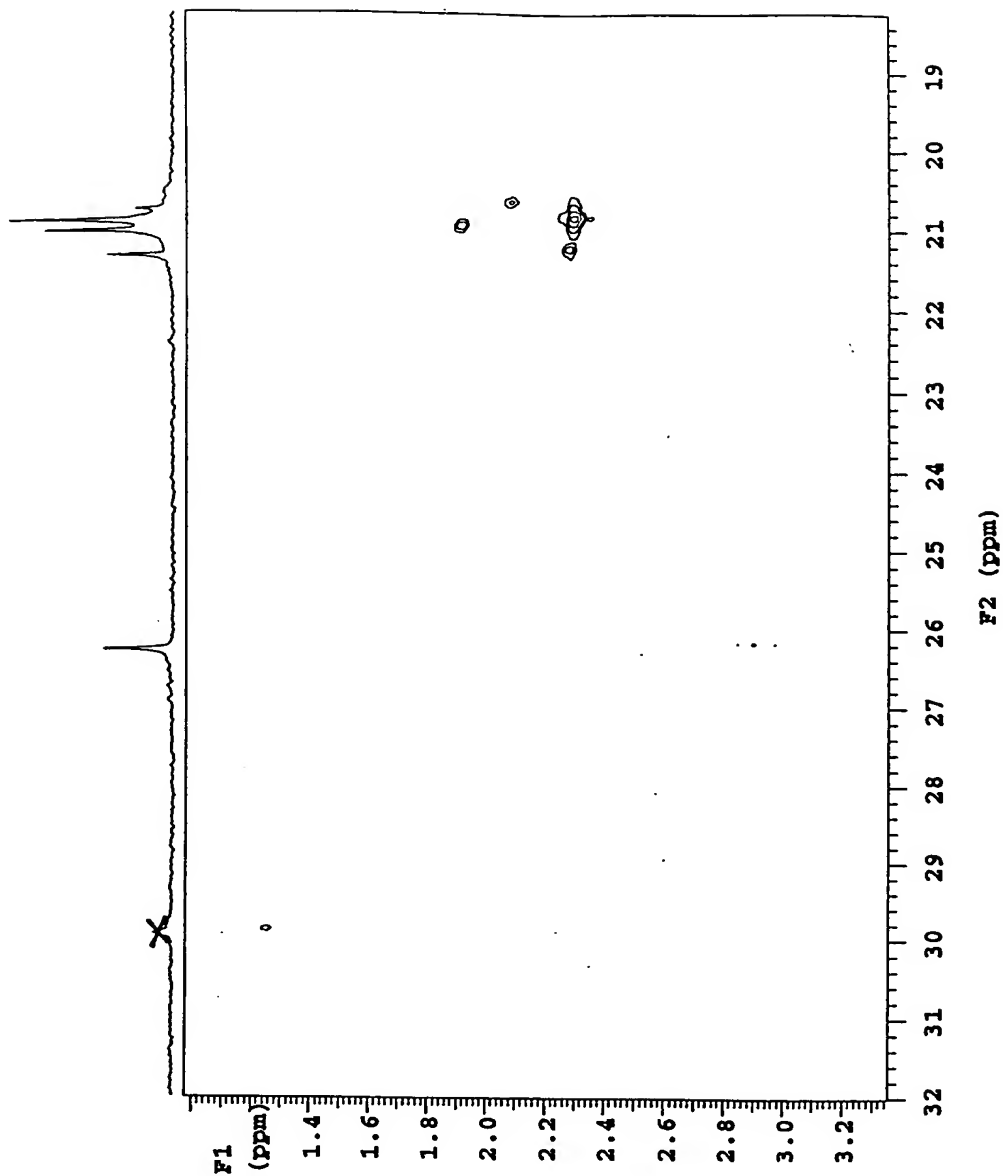


Fig. 28C

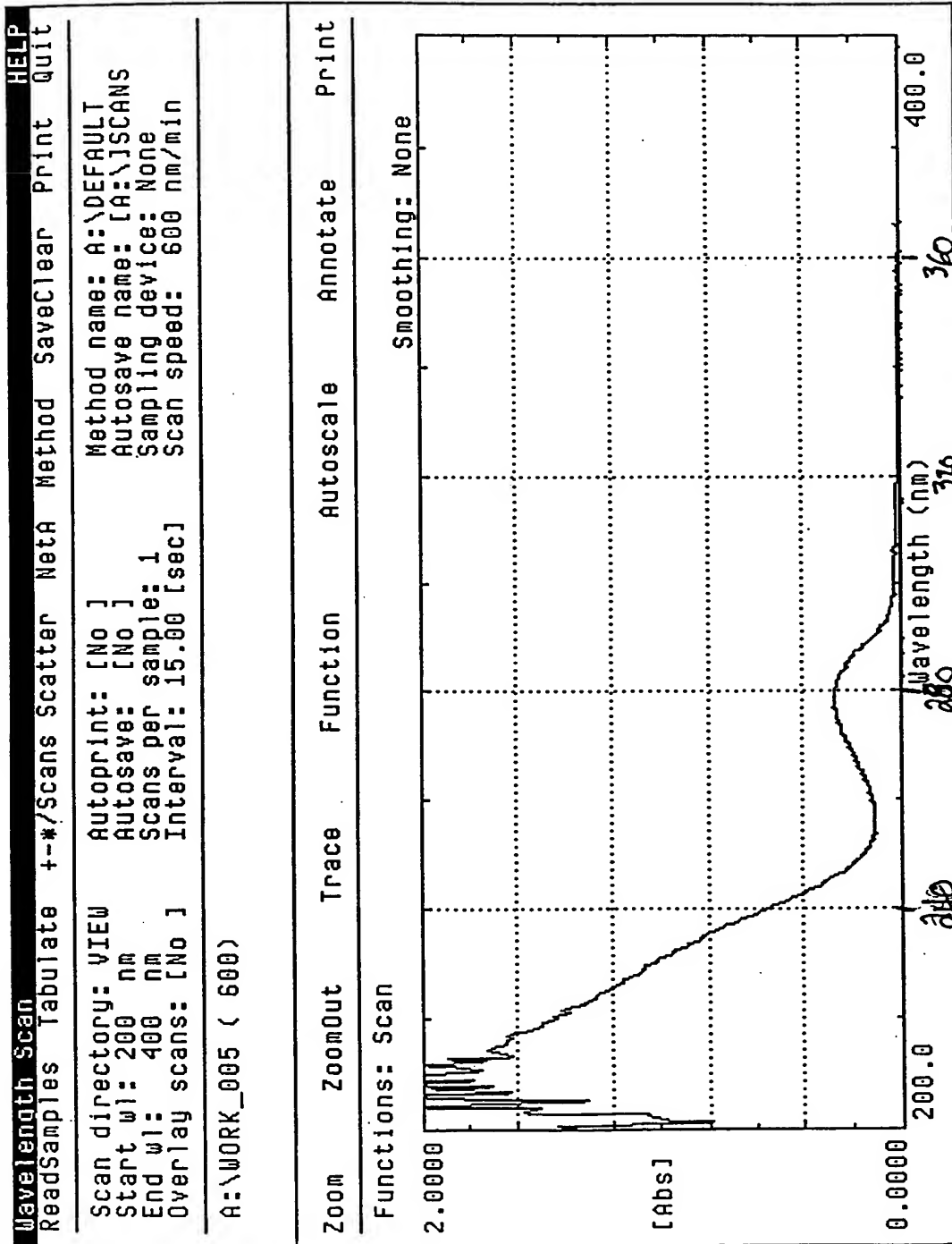


Fig. 29

36/40

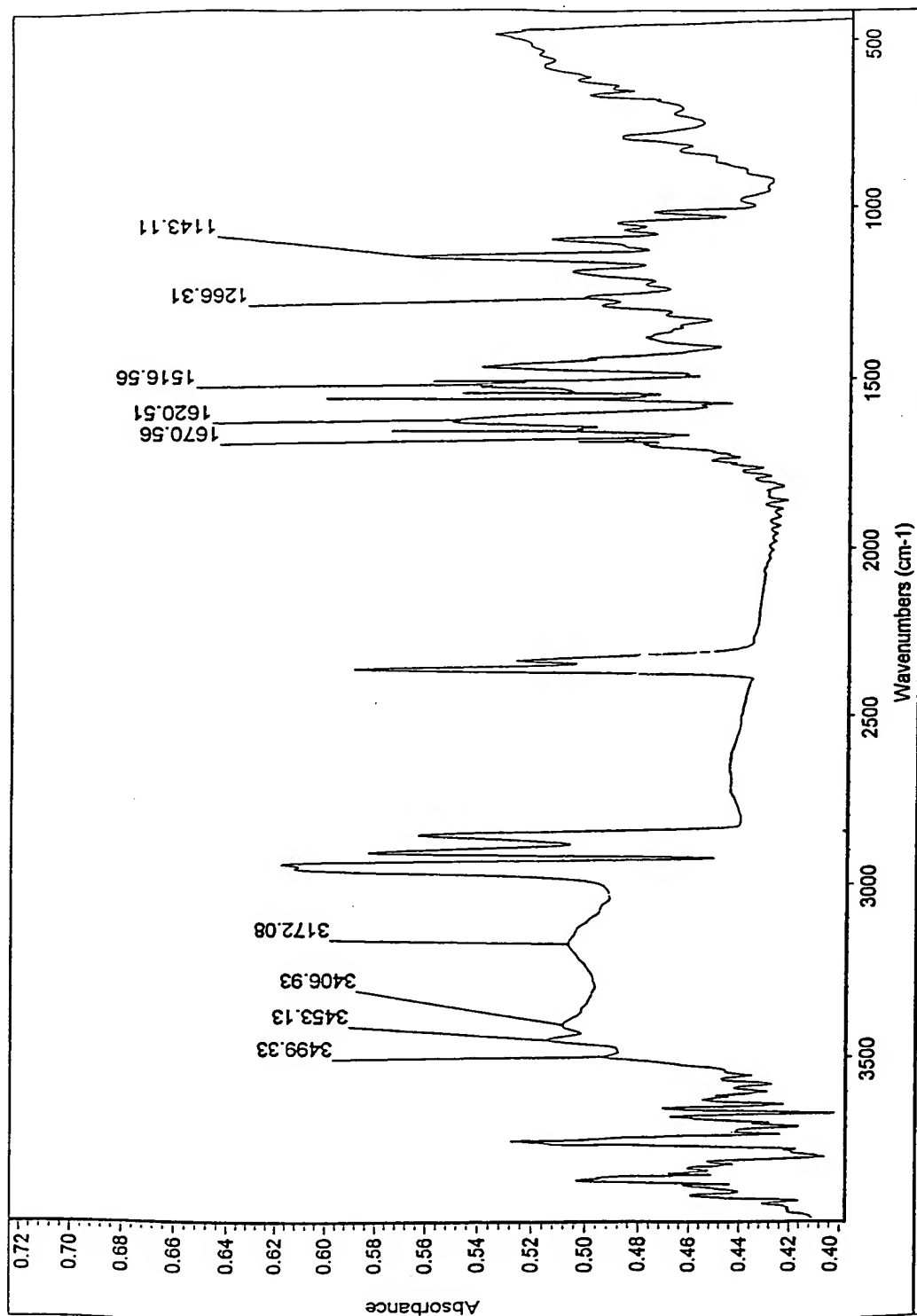


Fig. 30

\*\*Subtraction Result:proteotech, sampleL

Scans: 32

Resolution: 4.000

## Aromatic Alcohols and Phenols

Aldrich 85,523-5  
(-)-Epicatechin, 97%

CAS (490-46-0)

FT-IR:  $\nu$ , 11200

$C_{15}H_{14}O_6$   
FW 290.27  
mp 240°C d.

156.31 130.42 94.89\*  
156.01 117.76\* 83.91\*  
155.67 114.69\* 77.85\*  
144.28 114.58\* 64.75\*  
144.23 88.31 28.07

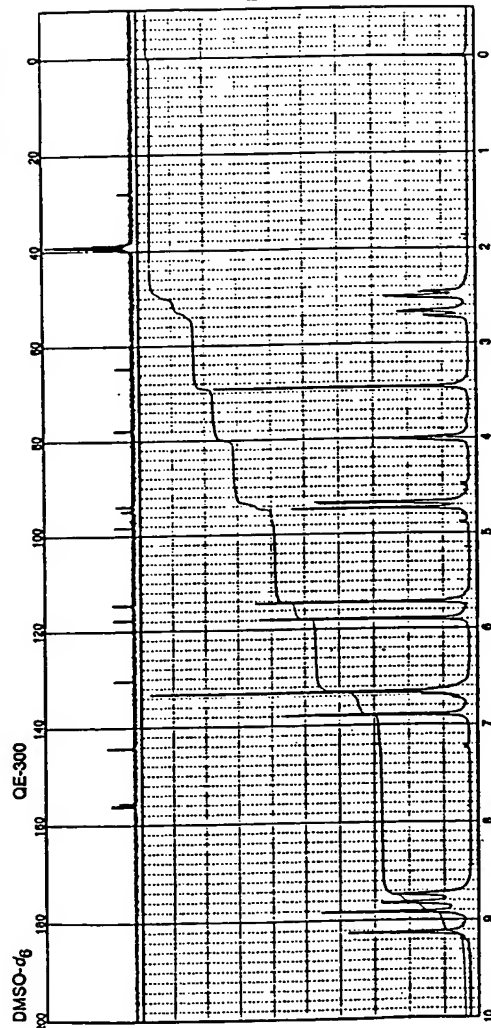


Fig. 31A

Aldrich 86,181-2  
(±)-Catechin hydrate, 98%

$C_{15}H_{14}O_6$   
FW 290.28  
mp 210°C d.

156.25 114.35\*  
155.87 88.90  
155.15 94.97\*  
144.65 83.70\*  
130.43 80.83\*  
118.24\* 66.17\*  
114.82\* 27.70

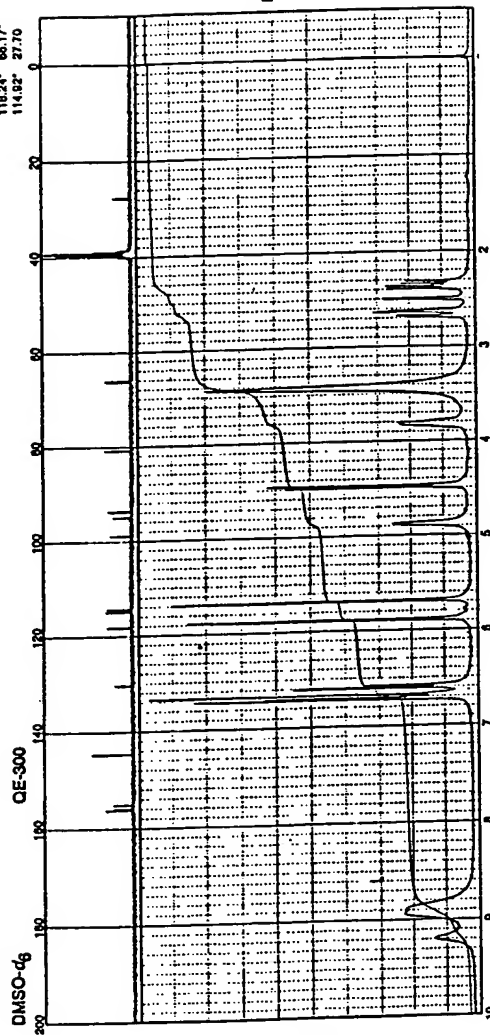


Fig. 31B

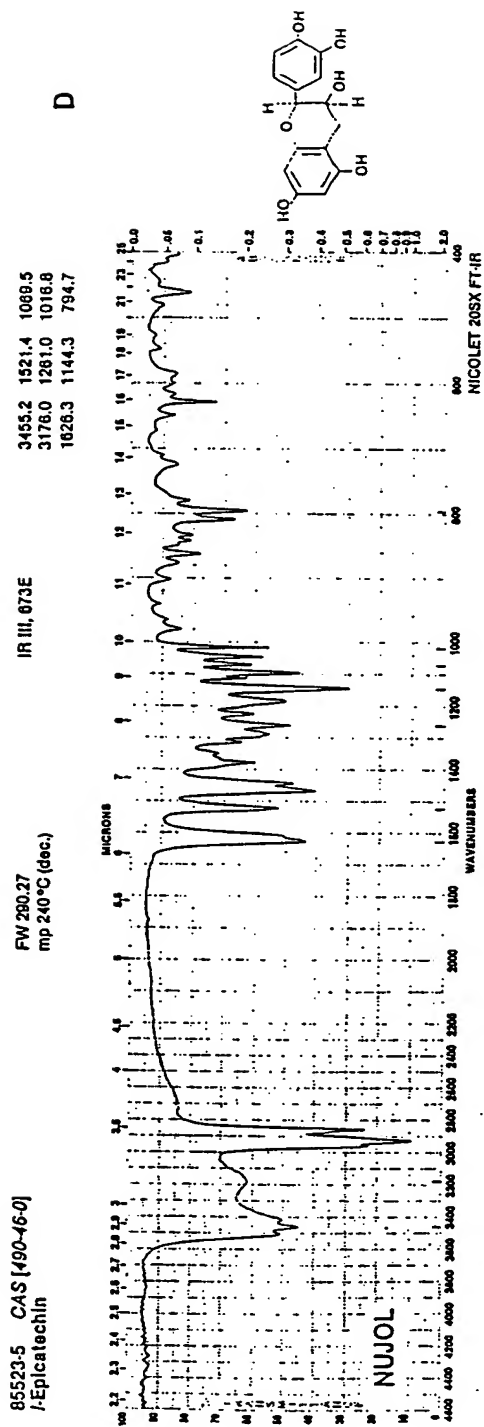


Fig. 32A

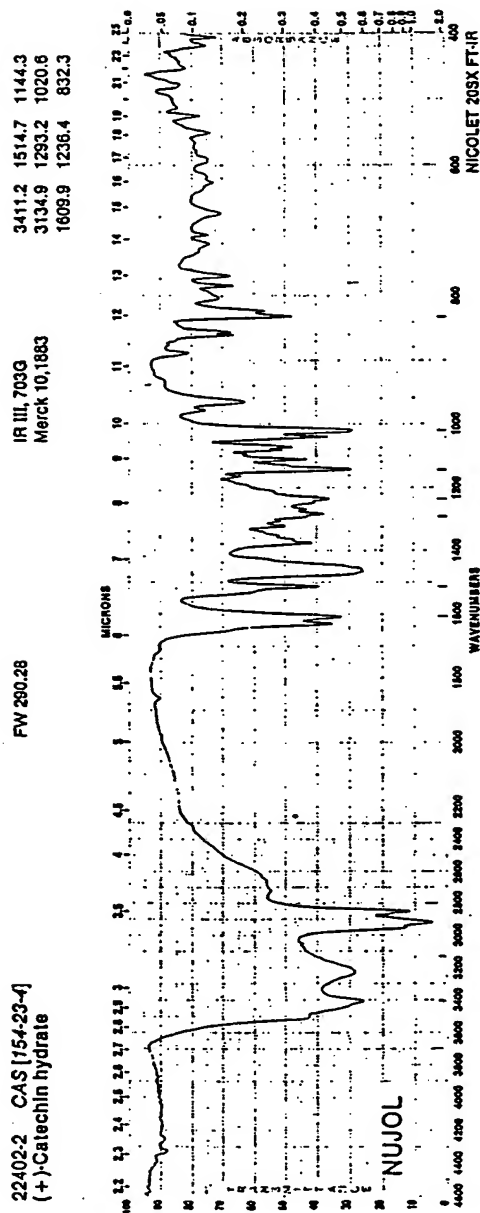


Fig. 32B

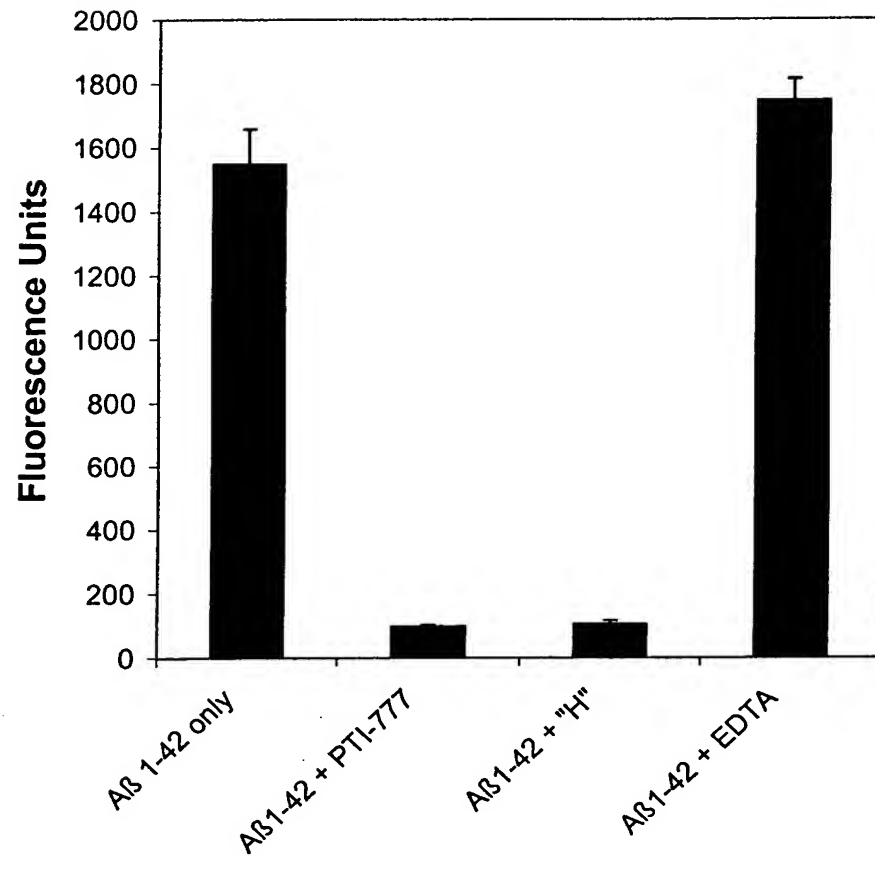


Fig. 33

40/40

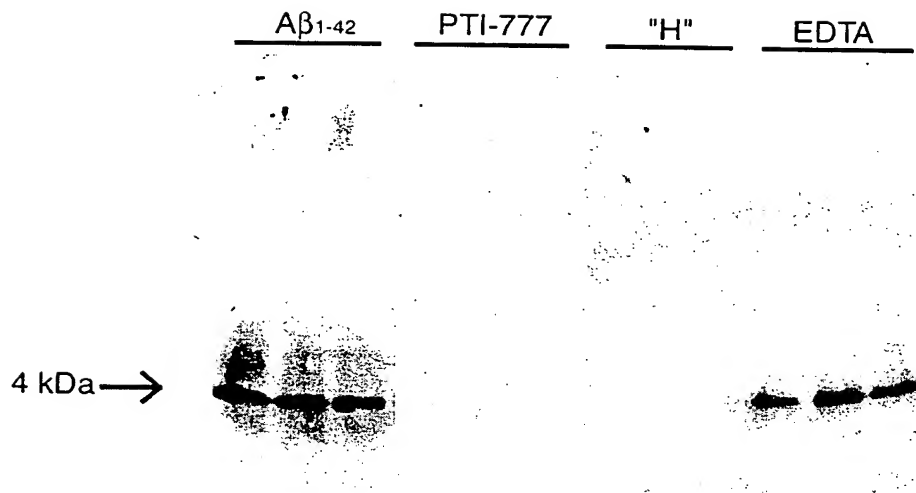


Fig. 34